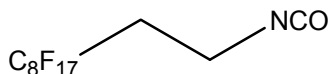


**F017032**

## 2-(Perfluorooctyl)ethyl isocyanate



Chemical Formula:	C <sub>11</sub> H <sub>4</sub> F <sub>17</sub> NO
Formula Weight:	489.13
Description:	Scavenger for nucleophiles
CAS Number:	142010-50-2
Appearance:	Low melting solid
Soluble in:	Methanol, THF, dichloromethane, ethyl acetate and acetone
Stability:	Store in brown bottle at ambient temperature

**DESCRIPTION AND USES:**

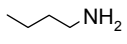
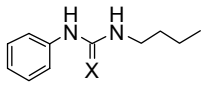
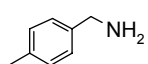
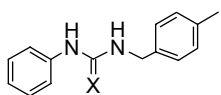
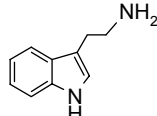
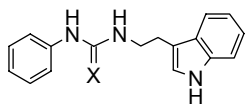
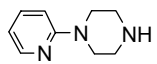
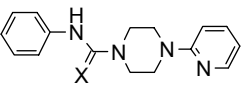
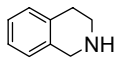
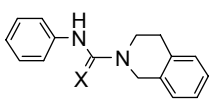
- Fluorous isocyanate is a solution-phase scavenger for nucleophiles.
- Used in solution-phase parallel synthesis of urea, thiourea and β-hydroxyamine analogs.<sup>1</sup>
- Resulting fluorinated-quenched derivatives were readily separated from the desired product by fluorinated solid-phase extractions (F-SPE) over FluoroFlash<sup>®</sup> cartridges to give products with good purity.<sup>2-4</sup>

**TYPICAL PROCEDURE:**

Typical procedure for the reaction of **1a** with amines: To a solution of phenyl isocyanate **1a** (1.0 equiv, 0.2 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (0.5-1.0 mL) was added an excess amount of amine (1.5 equiv, 0.3 mmol). The resulting solution was stirred at 60 °C for 6-12 h in a capped vial. Upon completion of the reaction, fluorinated isocyanate was added (1.0 equiv, 0.2 mmol) and the reaction mixture was stirred for 2.5 h at 60 °C. The reaction mixture was concentrated to 0.2-0.5 mL and loaded under vacuum onto a 5g FluoroFlash<sup>®</sup> SPE cartridge pre-conditioned with 80:20 MeOH-H<sub>2</sub>O on a SPE manifold. The cartridge was eluted with 10 mL of 80:20 MeOH-H<sub>2</sub>O. The MeOH-H<sub>2</sub>O fraction containing the desired product was evaporated in a Speedvac to give the corresponding urea **2a** in quantitative yield. The F-SPE cartridge can be reconditioned by first washing with 100% MeOH followed by THF or acetone to remove the fluorinated compounds from the cartridge and then re-equilibrated with 80:20 MeOH-H<sub>2</sub>O for the next round of F-SPE. The cartridge can typically be reused up to 10 times, depending on the nature of the substrate applied.



**Structures, yields, and purities of ureas and thioureas<sup>a</sup>**

substrate	amine	product	X	yield	purity <sup>a</sup>
<b>1a</b>			O	52%	95%
<b>1b</b>			S	98%	95%
<b>1a</b>			O	100%	>95%
<b>1b</b>			S	80%	>95%
<b>1a</b>			O	100%	95%
<b>1b</b>			S	34%	95%
<b>1a</b>			O	100%	95%
<b>1b</b>			S	68%	>95%
<b>1a</b>			O	100%	95%
<b>1b</b>			S	96%	95%

<sup>a</sup> Purity was assessed by <sup>1</sup>H NMR

**REFERENCES:**

- Zhang, W.; Chen, C. H.-T.; Nagashima, T. *Tetrahedron Lett.*, **2003**, 44, 2065-2068.
- For related scavenger work, see: (a) Lindsley, C. W.; Zhao, Z.; Leister, W. H. *Tetrahedron Lett.* **2002**, 43, 4225; (b) Lindsley, C. W.; Zhao, Z.; Leister, W. H.; Strauss, K. A. *Tetrahedron Lett.* **2002**, 43, 6319 (c) Zhang, W.; Curran, D. P.; Chen, C. H.-T. *Tetrahedron*, **2002**, 58, 3871.
- Curran, D. P. *Synlett*, **2001**, 1488.
- Please refer to FTI Application Note "Fluorous solid Phase Extraction"

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