

3-(Dimethylamino)ppropyl isothiocyanate

Inchi:	InChI=1S/C6H12N2S/c1-8(2)5-3-4-7-6-9/h3-5H2,1-2H3
InchiKey:	LDXHWJITNCSIJC-UHFFFAOYSA-N
Formula:	C6H12N2S
SMILES:	CN(C)CCCN=C=S
Mol. weight [g/mol]:	144.24

Physical Properties

Property code	Value	Unit	Source
ie	8.13	eV	Cheméo Relay (1.0)
logp	1.041		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
tb	465.70	K	Cheméo Relay (1.0)
tf	235.49	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C27421701&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/98-480-1/3-Dimethylamino-ppropyl-isothiocyanate.pdf>

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