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