3-Methylbutyl isothiocyanate

Other names: 3-Methylbutyl isothiocyanate
Inchi: InChI=1S/C6H11NS/c1-6(2)3-4-7-5-8/h6H,3-4H2,1-2H3
InchiKey: JATNWMBUDXLMEO-UHFFFAOYSA-N
Formula: C6H11NS
SMILES: CC(C)CCN=C=S
Mol. weight [g/mol]: 129.23

Physical Properties

Property code	Value	Unit	Source
hvap	45.01	kJ/mol	Cheméo Relay (1.0)
ie	8.93	eV	Cheméo Relay (1.0)
logp	2.135		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
rinpol	1040.70		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1040.70		NIST Webbook
ripol	1418.00		NIST Webbook

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C628035&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices