1-Pentane isothiocyanate

Other names:	Pentyl isothiocyanate
	n-Amyl isothiocyanate
	Pentane, 1-isothiocyanato-
Inchi:	InChI=1S/C6H11NS/c1-2-3-4-5-7-6-8/h2-5H2,1H3
InchiKey:	SGHJUJBYMSVAJY-UHFFFAOYSA-N
Formula:	C6H11NS
SMILES:	CCCCCN=C=S
Mol. weight [g/mol]:	129.23

Physical Properties

Property code	Value	Unit	Source
hvap	46.83	kJ/mol	Cheméo Relay (1.0)
ie	8.97	eV	Cheméo Relay (1.0)
logp	2.279		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
rinpol	1079.40		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1079.40		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1473.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1473.00		NIST Webbook
tb	443.70	K	Cheméo Relay (1.0)

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=C629129&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
tb:	Normal Boiling Point Temperature