Cyclopentyl isothiocyanate

Inchi: InChI=1S/C6H9NS/c8-5-7-6-3-1-2-4-6/h6H,1-4H2
InchiKey: PJOODZCPFADLCI-UHFFFAOYSA-N
Formula: C6H9NS
SMILES: S=C=NC1CCCC1
Mol. weight [g/mol]: 127.21
CAS: 33522-03-1

Physical Properties

Property code	Value	Unit	Source
hf	177.38	kJ/mol	Joback Method
hvap	39.65	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.032		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
tb	497.91	K	Joback Method
tc	749.33	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33522031&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature