Cyclopropane, isothiocyanato-

Other names: cyclopropyl isothiocyanate
Inchi: InChI=1S/C4H5NS/c6-3-5-4-1-2-4/h4H,1-2H2
InchiKey: JGFBQFKZKSSODQ-UHFFFAOYSA-N
Formula: C4H5NS
SMILES: S=C=NC1CC1
Mol. weight [g/mol]: 99.15
CAS: 56601-42-4

Physical Properties

Property code	Value	Unit	Source
hf	230.98	kJ/mol	Joback Method
hvap	34.85	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.252		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	443.61	K	Joback Method
tc	684.10	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56601424&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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