Isopropyl isothiocyanate

Other names: Propane, 2-isothiocyanato-
Inchi: InChI=1S/C4H7NS/c1-4(2)5-3-6/h4H,1-2H3
InchiKey: VHBFEIBMZHEWSX-UHFFFAOYSA-N
Formula: C4H7NS
SMILES: CC(C)N=C=S
Mol. weight [g/mol]: 101.17
CAS: 2253-73-8

Physical Properties

Property code	Value	Unit	Source
hf	152.90	kJ/mol	Joback Method
hvap	34.55	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.498		Crippen Method
mcvol	84.950	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
rinpol	835.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	817.90		NIST Webbook
rinpol	837.00		NIST Webbook
ripol	1177.00		NIST Webbook
tb	436.43	K	Joback Method
tc	662.78	K	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2253738&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature