1,3-Propane diisothiocyanate

Inchi: InChI=1S/C5H6N2S2/c8-4-6-2-1-3-7-5-9/h1-3H2
InchiKey: HSFDFWROECINQQ-UHFFFAOYSA-N
Formula: C5H6N2S2
SMILES: S=C=NCCCN=C=S
Mol. weight [g/mol]: 158.25
CAS: 52714-52-0

Physical Properties

Property code	Value	Unit	Source
hf	421.61	kJ/mol	Joback Method
hvap	47.60	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.582		Crippen Method
mcvol	116.770	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	605.70	K	Joback Method
tc	868.73	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=C52714520&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature