4-Isothiocyanatobenzenesulfonamide

Inchi: InChI=1S/C7H6N2O2S2/c8-13(10,11)7-3-1-6(2-4-7)9-5-12/h1-4H,(H2,8,10,11)
InchiKey: IMDUFDNFSJWYQT-UHFFFAOYSA-N
Formula: C7H6N2O2S2
SMILES: NS(=O)(=O)c1ccc(N=C=S)cc1
Mol. weight [g/mol]: 214.26
CAS: 51908-29-3

Physical Properties

Property code	Value	Unit	Source
hf	-98.24	kJ/mol	Joback Method
hvap	73.83	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.068		Crippen Method
mcvol	141.530	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method
tb	657.48	K	Joback Method
tc	917.29	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51908293&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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