1,2-Phenylene diisothiocyanate

Inchi: InChI=1S/C8H4N2S2/c11-5-9-7-3-1-2-4-8(7)10-6-12/h1-4H
InchiKey: RPFLVLIPBDQGAQ-UHFFFAOYSA-N
Formula: C8H4N2S2
SMILES: S=C=Nc1ccccc1N=C=S
Mol. weight [g/mol]: 192.26
CAS: 71105-17-4

Physical Properties

Property code	Value	Unit	Source
hf	584.75	kJ/mol	Joback Method
hvap	57.22	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.155		Crippen Method
mcvol	135.280	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	706.00	K	Joback Method
tc	1007.91	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71105174&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