Benzene, 2-chloro-4-isothiocyanato-1-methyl-

Inchi: InChI=1S/C8H6ClNS/c1-6-2-3-7(10-5-11)4-8(6)9/h2-4H,1H3
InchiKey: PQLHTYDGCDDPNU-UHFFFAOYSA-N
Formula: C8H6ClNS
SMILES: Cc1ccc(N=C=S)cc1Cl
Mol. weight [g/mol]: 183.66
CAS: 19241-37-3

Physical Properties

Property code	Value	Unit	Source
hf	273.47	kJ/mol	Joback Method
hvap	51.83	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.383		Crippen Method
mcvol	129.790	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	602.46	K	Joback Method
tc	868.07	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19241373&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