Benzene, 1,2,4-trichloro-5-isothiocyanato-

Other names: 2,4,5-trichlorophenyl isothiocyanate
Inchi: InChI=1S/C7H2Cl3NS/c8-4-1-6(10)7(11-3-12)2-5(4)9/h1-2H
InchiKey: PJLRSYLEFZNICX-UHFFFAOYSA-N
Formula: C7H2Cl3NS
SMILES: S=C=Nc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 238.52
CAS: 23165-46-0

Physical Properties

Property code	Value	Unit	Source
hf	251.16	kJ/mol	Joback Method
hvap	59.03	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.381		Crippen Method
mcvol	140.180	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	659.42	K	Joback Method
tc	938.05	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23165460&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