

Benzene, 1,3,5-trichloro-2-isothiocyanato-

Other names:	2,4,6-trichlorophenyl isothiocyanate
Inchi:	InChI=1S/C7H2Cl3NS/c8-4-1-5(9)7(11-3-12)6(10)2-4/h1-2H
InchiKey:	DSXVZIOQROMOEF-UHFFFAOYSA-N
Formula:	C7H2Cl3NS
SMILES:	S=C=Nc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	238.52
CAS:	22134-07-2

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

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=C22134072&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

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