

3,5-Dichlorophenyl isothiocyanate

Inchi:	InChI=1S/C7H3Cl2NS/c8-5-1-6(9)3-7(2-5)10-4-11/h1-3H
InchiKey:	JLEMKZDHFHGHLO-UHFFFAOYSA-N
Formula:	C7H3Cl2NS
SMILES:	S=C=Nc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	204.08
CAS:	6590-93-8

Physical Properties

Property code	Value	Unit	Source
hf	278.37	kJ/mol	Joback Method
hvap	53.99	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.728		Crippen Method
mcpvol	127.940	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	617.01	K	Joback Method
tc	892.29	K	Joback Method

Sources

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=C6590938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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