

3,5-Dichlorophenyl isocyanate

Other names:	Benzene, 1,3-dichloro-5-isocyanato- 1,3-dichloro-5-isocyanatobenzene
Inchi:	InChI=1S/C7H3Cl2NO/c8-5-1-6(9)3-7(2-5)10-4-11/h1-3H
InchiKey:	XEFUJGURFLOFAN-UHFFFAOYSA-N
Formula:	C7H3Cl2NO
SMILES:	O=C=Nc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	188.01
CAS:	34893-92-0

Physical Properties

Property code	Value	Unit	Source
hf	-11.11	kJ/mol	Joback Method
hvap	53.08	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	2.961		Crippen Method
mcvol	117.460	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	537.73	K	Joback Method
tc	775.74	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34893920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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