Benzene, 1,4-dichloro-2-isocyanato-

Other names: 2,5-Dichlorophenyl isocyanate
Isocyanic acid, 2,5-dichlorophenyl ester
Inchi: InChI=1S/C7H3Cl2NO/c8-5-1-2-6(9)7(3-5)10-4-11/h1-3H
InchiKey: PEQMJVGRHNZPAM-UHFFFAOYSA-N
Formula: C7H3Cl2NO
SMILES: O=C=Nc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 188.01
CAS: 5392-82-5

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

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=C5392825&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