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

Physical Properties

Property code	Value	Unit	Source
hf	-50.15	kJ/mol	Cheméo Relay (1.0)
hvap	57.38	kJ/mol	Cheméo Relay (1.0)
ie	9.05	eV	Cheméo Relay (1.0)
log10ws	-3.87		Cheméo Relay (1.0)
logp	2.961		Crippen Method
mcvol	117.460	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	486.70	K	Cheméo Relay (1.0)
tc	733.47	K	Cheméo Relay (1.0)
tf	328.35	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C34893920&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point