Benzene, 1-chloro-2-isocyanato-

Other names:	Isocyanic acid, o-chlorophenyl ester
	o-Chlorophenyl isocyanate
	2-Chlorophenyl isocyanate
Inchi:	InChI=1S/C7H4ClNO/c8-6-3-1-2-4-7(6)9-5-10/h1-4H
InchiKey:	NOHQUGRVHSJYMR-UHFFFAOYSA-N
Formula:	C7H4ClNO
SMILES:	O=C=Nc1ccccc1Cl
Mol. weight [g/mol]:	153.57
CAS:	3320-83-0

Physical Properties

Property code	Value	Unit	Source
chs	-3272.00 ± 4.20	kJ/mol	NIST Webbook
hf	16.10	kJ/mol	Joback Method
hfs	-74.50 ± 4.20	kJ/mol	NIST Webbook
hvap	48.03	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	2.307		Crippen Method
mcvol	105.220	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	495.32	K	Joback Method
tc	727.09	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=C3320830&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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