

4-Chloro-3-nitrophenyl isocyanate

Inchi: InChI=1S/C7H3ClN2O3/c8-6-2-1-5(9-4-11)3-7(6)10(12)13/h1-3H
InchiKey: ZCPHLSPLEGBTZ-UHFFFAOYSA-N
Formula: C7H3ClN2O3
SMILES: O=C=Nc1ccc(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 198.56
CAS: 40397-96-4

Physical Properties

Property code	Value	Unit	Source
hf	-6.13	kJ/mol	Joback Method
hvap	65.28	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	2.216		Crippen Method
mcvol	122.640	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
tb	652.14	K	Joback Method
tc	911.54	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=C40397964&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

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