

Cyclobutanecarboxamide, N-(3-chlorophenyl)-

Inchi: InChI=1S/C11H12ClNO/c12-9-5-2-6-10(7-9)13-11(14)8-3-1-4-8/h2,5-8H,1,3-4H2,(H,13,14)
InchiKey: NKTPEKDVZVAYNU-UHFFFAOYSA-N
Formula: C11H12ClNO
SMILES: OC(=Nc1cccc(Cl)c1)C1CCC1
Mol. weight [g/mol]: 209.67

Physical Properties

Property code	Value	Unit	Source
hf	-74.21	kJ/mol	Joback Method
hvap	67.56	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.728		Crippen Method
mcvol	155.020	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinsol	1872.00		NIST Webbook
rinsol	1872.00		NIST Webbook
tb	699.92	K	Joback Method
tc	932.35	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemed.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=U307048&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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