Cyclopentanecarboxamide, N-(3-chlorophenyl)-

Inchi: InChI=1S/C12H14ClNO/c13-10-6-3-7-11(8-10)14-12(15)9-4-1-2-5-9/h3,6-9H,1-2,4-5H2,(
InchiKey: YOKCBEZMIXZJTA-UHFFFAOYSA-N
Formula: C12H14ClNO
SMILES: O=C(Nc1cccc(Cl)c1)C1CCCC1
Mol. weight [g/mol]: 223.70

Physical Properties

Property code	Value	Unit	Source
gf	138.03	kJ/mol	Joback Method
hf	-80.32	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	63.07	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.469		Crippen Method
mcvol	169.110	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	1976.00		NIST Webbook
tb	662.37	K	Joback Method
tc	904.65	K	Joback Method
tf	407.35	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.28	J/mol×K	662.37	Joback Method
cpg	451.20	J/mol×K	702.75	Joback Method
cpg	465.87	J/mol×K	743.13	Joback Method
cpg	479.35	J/mol×K	783.51	Joback Method
cpg	491.71	J/mol×K	823.89	Joback Method
cpg	503.02	J/mol×K	864.27	Joback Method
cpg	513.36	J/mol×K	904.65	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=U307026&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume