Cyclohexanecarboxamide, N-(3-chlorophenyl)-

Inchi: InChI=1S/C13H16ClNO/c14-11-7-4-8-12(9-11)15-13(16)10-5-2-1-3-6-10/h4,7-10H,1-3,5-
InchiKey: WGUWTOYIQWKLDD-UHFFFAOYSA-N
Formula: C13H16ClNO
SMILES: O=C(Nc1cccc(Cl)c1)C1CCCCC1
Mol. weight [g/mol]: 237.72

Physical Properties

Property code	Value	Unit	Source
gf	134.35	kJ/mol	Joback Method
hf	-107.12	kJ/mol	Joback Method
hfus	25.81	kJ/mol	Joback Method
hvap	65.47	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.859		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	2070.00		NIST Webbook
tb	689.52	K	Joback Method
tc	934.43	K	Joback Method
tf	415.10	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.28	J/mol×K	689.52	Joback Method
cpg	506.42	J/mol×K	730.34	Joback Method
cpg	522.16	J/mol×K	771.16	Joback Method
cpg	536.57	J/mol×K	811.98	Joback Method
cpg	549.73	J/mol×K	852.80	Joback Method
cpg	561.68	J/mol×K	893.61	Joback Method
cpg	572.51	J/mol×K	934.43	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=U306947&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