1-(4-Chlorophenyl)-1-cyclohexane-carboxylic acid

Other names: 1-(4-Chlorophenyl)cyclohexane-1-carboxylic acid
Cyclohexanecarboxylic acid, 1-(4-chlorophenyl)-
1-(4-chlorophenyl)cyclohexanecarboxylic acid
Inchi: InChI=1S/C13H15ClO2/c14-11-6-4-10(5-7-11)13(12(15)16)8-2-1-3-9-13/h4-7H,1-3,8-9H2
InchiKey: UPNXUJXIIZGXLQ-UHFFFAOYSA-N
Formula: C13H15ClO2
SMILES: O=C(O)C1(c2ccc(Cl)cc2)CCCCC1
Mol. weight [g/mol]: 238.71
CAS: 58880-37-8

Physical Properties

Property code	Value	Unit	Source
gf	-97.35	kJ/mol	Joback Method
hf	-297.58	kJ/mol	Joback Method
hfus	18.50	kJ/mol	Joback Method
hvap	74.56	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.627		Crippen Method
mcvol	179.090	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	731.77	K	Joback Method
tc	966.51	K	Joback Method
tf	447.16	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.27	J/mol×K	731.77	Joback Method
cpg	501.57	J/mol×K	770.89	Joback Method
cpg	515.18	J/mol×K	810.02	Joback Method
cpg	528.26	J/mol×K	849.14	Joback Method
cpg	540.98	J/mol×K	888.27	Joback Method
cpg	553.51	J/mol×K	927.39	Joback Method

cpg	566.01	J/mol×K	966.51	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=C58880378&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume