1-(4-Chlorophenyl)cyclohexane-1-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

Physical Properties

Property code	Value	Unit	Source
hfus	18.50	kJ/mol	Joback Method
logp	3.627		Crippen Method
mcvol	179.090	ml/mol	McGowan 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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58880378&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume