1-(4-Methoxyphenyl)-1-cyclohexanecarboxylic acid

Other names: Cyclohexanecarboxylic acid, 1-(4-methoxyphenyl)-
1-(4-methoxyphenyl)cyclohexane-1-carboxylic acid
Inchi: InChI=1S/C14H18O3/c1-17-12-7-5-11(6-8-12)14(13(15)16)9-3-2-4-10-14/h5-8H,2-4,9-10
InchiKey: JKJAJSWMKTWWJS-UHFFFAOYSA-N
Formula: C14H18O3
SMILES: COc1ccc(C2(C(=O)O)CCCCC2)cc1
Mol. weight [g/mol]: 234.29
CAS: 7469-83-2

Physical Properties

Property code	Value	Unit	Source
gf	-182.00	kJ/mol	Joback Method
hf	-434.70	kJ/mol	Joback Method
hfus	18.08	kJ/mol	Joback Method
hvap	74.81	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.982		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	739.64	K	Joback Method
tc	964.74	K	Joback Method
tf	450.74	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.54	J/mol×K	739.64	Joback Method
cpg	557.08	J/mol×K	777.16	Joback Method
cpg	571.89	J/mol×K	814.67	Joback Method
cpg	586.08	J/mol×K	852.19	Joback Method
cpg	599.81	J/mol×K	889.70	Joback Method
cpg	613.18	J/mol×K	927.22	Joback Method
cpg	626.34	J/mol×K	964.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7469832&Units=SI
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

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