4-Cyclohexylphenylacetic acid

Inchi: InChI=1S/C14H18O2/c15-14(16)10-11-6-8-13(9-7-11)12-4-2-1-3-5-12/h6-9,12H,1-5,10H2
InchiKey: ZHMWKJWMWIWEPJ-UHFFFAOYSA-N
Formula: C14H18O2
SMILES: O=C(O)Cc1ccc(C2CCCCC2)cc1
Mol. weight [g/mol]: 218.29
CAS: 35889-00-0

Physical Properties

Property code	Value	Unit	Source
gf	-71.51	kJ/mol	Joback Method
hf	-317.72	kJ/mol	Joback Method
hfus	23.19	kJ/mol	Joback Method
hvap	73.55	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.361		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1940.00		NIST Webbook
rinpol	1940.00		NIST Webbook
tb	716.98	K	Joback Method
tc	937.39	K	Joback Method
tf	404.61	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.34	J/mol×K	716.98	Joback Method
cpg	534.94	J/mol×K	753.72	Joback Method
cpg	549.41	J/mol×K	790.45	Joback Method
cpg	562.80	J/mol×K	827.19	Joback Method
cpg	575.17	J/mol×K	863.92	Joback Method
cpg	586.55	J/mol×K	900.66	Joback Method
cpg	597.00	J/mol×K	937.39	Joback Method

dvisc	0.0024829	Pa×s	404.61	Joback Method
dvisc	0.0008752	Pa×s	456.67	Joback Method
dvisc	0.0003819	Pa×s	508.73	Joback Method
dvisc	0.0001944	Pa×s	560.80	Joback Method
dvisc	0.0001110	Pa×s	612.86	Joback Method
dvisc	0.0000692	Pa×s	664.92	Joback Method
dvisc	0.0000462	Pa×s	716.98	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=C35889000&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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