Cyclohexylphenylacetic acid

Other names: «alpha»-Cyclohexylphenylacetic acid
Benzeneacetic acid, «alpha»-cyclohexyl-
Inchi: InChI=1S/C14H18O2/c15-14(16)13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1,3-4,7-8,12-13H
InchiKey: AAJLPPDFIRPBDA-UHFFFAOYSA-N
Formula: C14H18O2
SMILES: O=C(O)C(c1ccccc1)C1CCCCC1
Mol. weight [g/mol]: 218.29
CAS: 3894-09-5

Physical Properties

Property code	Value	Unit	Source
gf	-64.32	kJ/mol	Joback Method
hf	-311.53	kJ/mol	Joback Method
hfus	20.06	kJ/mol	Joback Method
hvap	72.50	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.435		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
tb	711.56	K	Joback Method
tc	935.19	K	Joback Method
tf	415.70 ± 1.50	K	NIST Webbook
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.72	J/mol×K	711.56	Joback Method
cpg	536.78	J/mol×K	748.83	Joback Method
cpg	551.63	J/mol×K	786.10	Joback Method
cpg	565.33	J/mol×K	823.37	Joback Method
cpg	577.94	J/mol×K	860.65	Joback Method
cpg	589.51	J/mol×K	897.92	Joback Method
cpg	600.10	J/mol×K	935.19	Joback Method

dvisc	0.0048802	Pa×s	377.09	Joback Method
dvisc	0.0013374	Pa×s	432.84	Joback Method
dvisc	0.0004925	Pa×s	488.58	Joback Method
dvisc	0.0002225	Pa×s	544.33	Joback Method
dvisc	0.0001165	Pa×s	600.07	Joback Method
dvisc	0.0000681	Pa×s	655.81	Joback Method
dvisc	0.0000433	Pa×s	711.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3894095&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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