Benzeneacetic acid, «alpha»-cyclopentyl-

Other names:	«alpha»-Phenylcyclopentaneacetic acid
	Cyclopentylphenylacetic acid
	«alpha»-Cyclopentylphenylacetic acid
	Acetic acid, cyclopentylphenyl-
	Acetic acid, cyclopentyphenyl-
	Cyclopentaneacetic acid, «alpha»-phenyl-
Inchi:	InChI=1S/C13H16O2/c14-13(15)12(11-8-4-5-9-11)10-6-2-1-3-7-10/h1-3,6-7,11-12H,4-5,8
InchiKey:	BCJIDGDYYYBNNB-UHFFFAOYSA-N
Formula:	C13H16O2
SMILES:	O=C(O)C(c1ccccc1)C1CCCC1
Mol. weight [g/mol]:	204.26
CAS:	3900-93-4

Physical Properties

Property code	Value	Unit	Source
gf	-60.64	kJ/mol	Joback Method
hf	-284.73	kJ/mol	Joback Method
hfus	19.57	kJ/mol	Joback Method
hvap	70.10	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	3.045		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	684.41	K	Joback Method
tc	905.25	K	Joback Method
tf	369.34	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.32	J/mol×K	684.41	Joback Method
cpg	530.13	J/mol×K	868.44	Joback Method
cpg	519.11	J/mol×K	831.64	Joback Method

cpg	507.19	J/mol×K	794.83	Joback Method
cpg	494.29	J/mol×K	758.02	Joback Method
cpg	480.35	J/mol×K	721.22	Joback Method
cpg	540.30	J/mol×K	905.25	Joback Method
dvisc	0.0000710	Pa×s	684.41	Joback Method
dvisc	0.0001083	Pa×s	631.90	Joback Method
dvisc	0.0001785	Pa×s	579.39	Joback Method
dvisc	0.0003249	Pa×s	526.88	Joback Method
dvisc	0.0006754	Pa×s	474.36	Joback Method
dvisc	0.0016843	Pa×s	421.85	Joback Method
dvisc	0.0054467	Pa×s	369.34	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3900934&Units=SI

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

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