5-Hydroxy-5-methyl-2-phenylhexanoic acid

Inchi: InChI=1S/C13H18O3/c1-13(2,16)9-8-11(12(14)15)10-6-4-3-5-7-10/h3-7,11,16H,8-9H2,1-
InchiKey: TUGVMPVCGJMFKT-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: CC(C)(O)CCC(C(=O)O)c1ccccc1
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
gf	-231.17	kJ/mol	Joback Method
hf	-506.19	kJ/mol	Joback Method
hfus	22.31	kJ/mol	Joback Method
hvap	85.23	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.406		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1674.40		NIST Webbook
rinpol	1674.40		NIST Webbook
tb	758.08	K	Joback Method
tc	955.08	K	Joback Method
tf	421.68	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.34	J/mol×K	758.08	Joback Method
cpg	543.51	J/mol×K	790.91	Joback Method
cpg	553.95	J/mol×K	823.75	Joback Method
cpg	563.72	J/mol×K	856.58	Joback Method
cpg	572.87	J/mol×K	889.41	Joback Method
cpg	581.46	J/mol×K	922.25	Joback Method
cpg	589.54	J/mol×K	955.08	Joback Method
dvisc	0.0022793	Pa×s	421.68	Joback Method

dvisc	0.0004889	Pa×s	477.75	Joback Method
dvisc	0.0001449	Pa×s	533.81	Joback Method
dvisc	0.0000541	Pa×s	589.88	Joback Method
dvisc	0.0000240	Pa×s	645.95	Joback Method
dvisc	0.0000121	Pa×s	702.01	Joback Method
dvisc	0.0000068	Pa×s	758.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414860&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
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