3-Hydroxy-3-phenylvaleric acid

Inchi: InChI=1S/C11H14O3/c1-2-11(14,8-10(12)13)9-6-4-3-5-7-9/h3-7,14H,2,8H2,1H3,(H,12,13
InchiKey: AABQFWMUVKJALN-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CCC(O)(CC(=O)O)c1ccccc1
Mol. weight [g/mol]: 194.23
CAS: 13278-26-7

Physical Properties

Property code	Value	Unit	Source
gf	-245.57	kJ/mol	Joback Method
hf	-459.63	kJ/mol	Joback Method
hfus	20.65	kJ/mol	Joback Method
hvap	81.16	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.759		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
tb	712.76	K	Joback Method
tc	909.67	K	Joback Method
tf	414.14	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.95	J/mol×K	712.76	Joback Method
cpg	471.55	J/mol×K	876.85	Joback Method
cpg	463.98	J/mol×K	844.03	Joback Method
cpg	455.88	J/mol×K	811.22	Joback Method
cpg	447.21	J/mol×K	778.40	Joback Method
cpg	437.91	J/mol×K	745.58	Joback Method
cpg	478.65	J/mol×K	909.67	Joback Method
dvisc	0.0000116	Pa×s	712.76	Joback Method
dvisc	0.0000203	Pa×s	662.99	Joback Method

dvisc	0.0000390	Pa×s	613.22	Joback Method
dvisc	0.0000837	Pa×s	563.45	Joback Method
dvisc	0.0002083	Pa×s	513.68	Joback Method
dvisc	0.0006309	Pa×s	463.91	Joback Method
dvisc	0.0024937	Pa×s	414.14	Joback Method

Sources

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=C13278267&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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