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

Physical Properties

Property code	Value	Unit	Source
hfus	20.65	kJ/mol	Joback Method
hvap	101.50	kJ/mol	Cheméo Relay (1.0)
ie	8.77	eV	Cheméo Relay (1.0)
log10ws	-1.01		Cheméo Relay (1.0)
logp	1.759		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
tb	558.02	K	Cheméo Relay (1.0)
tf	382.32	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.95	J/mol×K	712.76	Joback Method
cpg	478.65	J/mol×K	909.67	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
dvisc	0.0000837	Pa×s	563.45	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	0.0024937	Pa×s	414.14	Joback Method
dvisc	0.0002083	Pa×s	513.68	Joback Method
dvisc	0.0006309	Pa×s	463.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13278267&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point