

2-Methyl-2-phenyl-3-hydroxypropanoic acid

Inchi:	InChI=1S/C10H12O3/c1-10(7-11,9(12)13)8-5-3-2-4-6-8/h2-6,11H,7H2,1H3,(H,12,13)
InchiKey:	ISSYFABJJSOCQG-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	CC(CO)(C(=O)O)c1ccccc1
Mol. weight [g/mol]:	180.20
CAS:	4370-81-4

Physical Properties

Property code	Value	Unit	Source
gf	-253.99	kJ/mol	Joback Method
hf	-438.99	kJ/mol	Joback Method
hfus	18.06	kJ/mol	Joback Method
hvap	78.94	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	1.021		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
tb	689.88	K	Joback Method
tc	888.69	K	Joback Method
tf	402.87	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.94	J/mol×K	689.88	Joback Method
cpg	418.69	J/mol×K	855.56	Joback Method
cpg	411.66	J/mol×K	822.42	Joback Method
cpg	404.12	J/mol×K	789.29	Joback Method
cpg	396.01	J/mol×K	756.15	Joback Method
cpg	387.30	J/mol×K	723.02	Joback Method
cpg	425.26	J/mol×K	888.69	Joback Method
dvisc	0.0000147	Pa×s	689.88	Joback Method
dvisc	0.0000258	Pa×s	642.05	Joback Method

dvisc	0.0000496	Pa×s	594.21	Joback Method
dvisc	0.0001070	Pa×s	546.38	Joback Method
dvisc	0.0002672	Pa×s	498.54	Joback Method
dvisc	0.0008102	Pa×s	450.70	Joback Method
dvisc	0.0031978	Pa×s	402.87	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=C4370814&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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