

Benzenepropanoic acid, «alpha»-hydroxy-, (S)-

Other names:	L-(-)-3-phenyllactic acid «alpha»-Hydroxyphenylpropanoic acid
Inchi:	InChI=1S/C9H10O3/c10-8(9(11)12)6-7-4-2-1-3-5-7/h1-5,8,10H,6H2,(H,11,12)
InchiKey:	VOXXWSYKYCBWHO-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	O=C(O)C(O)Cc1ccccc1
Mol. weight [g/mol]:	166.17
CAS:	20312-36-1

Physical Properties

Property code	Value	Unit	Source
gf	-267.69	kJ/mol	Joback Method
hf	-414.88	kJ/mol	Joback Method
hfus	19.36	kJ/mol	Joback Method
hvap	77.62	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.675		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
rinpol	1545.00		NIST Webbook
rinpol	1545.00		NIST Webbook
tb	669.79	K	Joback Method
tc	864.81	K	Joback Method
tf	374.18	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.39	J/mol×K	669.79	Joback Method
cpg	335.08	J/mol×K	702.29	Joback Method
cpg	343.21	J/mol×K	734.80	Joback Method
cpg	350.81	J/mol×K	767.30	Joback Method
cpg	357.90	J/mol×K	799.80	Joback Method

cpg	364.51	J/mol×K	832.31	Joback Method
cpg	370.66	J/mol×K	864.81	Joback Method
dvisc	0.0065458	Pa×s	374.18	Joback Method
dvisc	0.0014200	Pa×s	423.45	Joback Method
dvisc	0.0004236	Pa×s	472.72	Joback Method
dvisc	0.0001588	Pa×s	521.99	Joback Method
dvisc	0.0000705	Pa×s	571.25	Joback Method
dvisc	0.0000356	Pa×s	620.52	Joback Method
dvisc	0.0000199	Pa×s	669.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20312361&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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