L-(-)-2-HYDROXY-3-PHENYLPROPIONIC ACID

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]: 166.18

Physical Properties

Property code	Value	Unit	Source
af	0.7910		Cheméo Relay (1.0)
hf	-488.42	kJ/mol	Cheméo Relay (1.0)
hfus	19.36	kJ/mol	Joback Method
hvap	95.12	kJ/mol	Cheméo Relay (1.0)
ie	9.15	eV	Cheméo Relay (1.0)
log10ws	-0.28		Cheméo Relay (1.0)
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	548.74	K	Cheméo Relay (1.0)
tc	806.02	K	Cheméo Relay (1.0)
tf	346.13	K	Cheméo Relay (1.0)
vc	0.454	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20312361&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
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
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume