Atrolactic acid

Other names:	Benzeneacetic acid, «alpha»-hydroxy-«alpha»-methyl-
	Mandelic acid, «alpha»-methyl-
	«alpha»-Hydroxy-«alpha»-phenylpropionic acid
	«alpha»-Phenyllactic acid
	2-Hydroxy-2-phenylpropionic acid
	2-Phenyl-2-hydroxypropionic acid
	2-Phenyllactic acid
	dl-Atrolactic acid
	2-Hydroxy-2-phenylpropanoic acid
	DL-2-Phenyllactic acid
	DL-«alpha»-Phenyllactic acid
	NSC 128998
	NSC 401846
Inchi:	InChI=1S/C9H10O3/c1-9(12,8(10)11)7-5-3-2-4-6-7/h2-6,12H,1H3,(H,10,11)
InchiKey:	NWCHELUCVWSRRS-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	CC(O)(C(=O)O)c1ccccc1
Mol. weight [g/mol]:	166.17
CAS:	515-30-0

Physical Properties

Property code	Value	Unit	Source
gf	-262.41	kJ/mol	Joback Method
hf	-418.35	kJ/mol	Joback Method
hfus	15.47	kJ/mol	Joback Method
hvap	76.71	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	0.979		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
tb	667.00	K	Joback Method
tc	868.13	K	Joback Method
tf	391.60	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.29	J/mol×K	667.00	Joback Method
cpg	366.90	J/mol×K	834.61	Joback Method
cpg	360.46	J/mol×K	801.09	Joback Method
cpg	353.53	J/mol×K	767.56	Joback Method
cpg	346.05	J/mol×K	734.04	Joback Method
cpg	337.99	J/mol×K	700.52	Joback Method
cpg	372.89	J/mol×K	868.13	Joback Method
dvisc	0.0000186	Pa×s	667.00	Joback Method
dvisc	0.0000328	Pa×s	621.10	Joback Method
dvisc	0.0000634	Pa×s	575.20	Joback Method
dvisc	0.0001371	Pa×s	529.30	Joback Method
dvisc	0.0003432	Pa×s	483.40	Joback Method
dvisc	0.0010421	Pa×s	437.50	Joback Method
dvisc	0.0041052	Pa×s	391.60	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C515300&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume