Benzeneacetic acid, «alpha»,4-dihydroxy-3-methoxy-, methyl ester

Other names:	Mandelic acid, 4-hydroxy-3-methoxy-, methyl ester
	Methyl hydroxy(4-hydroxy-3-methoxyphenyl)acetate
Inchi:	InChI=1S/C10H12O5/c1-14-8-5-6(3-4-7(8)11)9(12)10(13)15-2/h3-5,9,11-12H,1-2H3
InchiKey:	XPQNHALAUGGUJN-UHFFFAOYSA-N
Formula:	C10H12O5
SMILES:	COC(=O)C(O)c1ccc(O)c(OC)c1
Mol. weight [g/mol]:	212.20
CAS:	2911-74-2

Physical Properties

Property code	Value	Unit	Source
gf	-496.70	kJ/mol	Joback Method
hf	-736.51	kJ/mol	Joback Method
hfus	25.63	kJ/mol	Joback Method
hvap	81.66	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	0.607		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
rinpol	1709.40		NIST Webbook
tb	730.93	K	Joback Method
tc	941.28	K	Joback Method
tf	493.33	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.10	J/mol×K	730.93	Joback Method
cpg	428.88	J/mol×K	765.99	Joback Method
cpg	438.09	J/mol×K	801.05	Joback Method
cpg	446.77	J/mol×K	836.11	Joback Method
cpg	454.95	J/mol×K	871.16	Joback Method
cpg	462.68	J/mol×K	906.22	Joback Method

cpg	469.97	J/mol×K	941.28	Joback Method
dvisc	0.0001497	Pa×s	493.33	Joback Method
dvisc	0.0000607	Pa×s	532.93	Joback Method
dvisc	0.0000279	Pa×s	572.53	Joback Method
dvisc	0.0000142	Pa×s	612.13	Joback Method
dvisc	0.0000078	Pa×s	651.73	Joback Method
dvisc	0.0000046	Pa×s	691.33	Joback Method
dvisc	0.0000029	Pa×s	730.93	Joback Method

Sources

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=C2911742&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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