Mandelic acid, 3,4-dimethoxy-, methyl ester

Other names:	Methyl «alpha»-hydroxy-«alpha»-(3,4-dimethoxyphenyl)acetate
	Methyl (3,4-dimethoxyphenyl)(hydroxy)acetate
Inchi:	InChI=1S/C11H14O5/c1-14-8-5-4-7(6-9(8)15-2)10(12)11(13)16-3/h4-6,10,12H,1-3H3
InchiKey:	GLMSKFAHFLOMQJ-UHFFFAOYSA-N
Formula:	C11H14O5
SMILES:	COC(=O)C(O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]:	226.23
CAS:	2911-73-1

Physical Properties

Property code	Value	Unit	Source
gf	-448.29	kJ/mol	Joback Method
hf	-723.53	kJ/mol	Joback Method
hfus	23.24	kJ/mol	Joback Method
hvap	73.95	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	0.910		Crippen Method
mcvol	167.140	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1700.10		NIST Webbook
rinpol	1686.00		NIST Webbook
tb	700.59	K	Joback Method
tc	899.06	K	Joback Method
tf	427.63	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.69	J/mol×K	700.59	Joback Method
cpg	498.24	J/mol×K	865.98	Joback Method
cpg	489.52	J/mol×K	832.90	Joback Method
cpg	480.09	J/mol×K	799.82	Joback Method
cpg	469.97	J/mol×K	766.75	Joback Method

cpg	459.16	J/mol×K	733.67	Joback Method
cpg	506.22	J/mol×K	899.06	Joback Method
dvisc	0.0000281	Pa×s	700.59	Joback Method
dvisc	0.0000403	Pa×s	655.10	Joback Method
dvisc	0.0000611	Pa×s	609.60	Joback Method
dvisc	0.0000990	Pa×s	564.11	Joback Method
dvisc	0.0001745	Pa×s	518.62	Joback Method
dvisc	0.0003432	Pa×s	473.12	Joback Method
dvisc	0.0007793	Pa×s	427.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2911731&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

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