3-Hydroxymandelic acid, dimethyl ether, methyl ester

Other names: Methyl methoxy(3-methoxyphenyl)acetate
Inchi: InChI=1S/C11H14O4/c1-13-9-6-4-5-8(7-9)10(14-2)11(12)15-3/h4-7,10H,1-3H3
InchiKey: PRJJVJQUMHDYMQ-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: COC(=O)C(OC)c1cccc(OC)c1
Mol. weight [g/mol]: 210.23

Physical Properties

Property code	Value	Unit	Source
gf	-301.84	kJ/mol	Joback Method
hf	-559.83	kJ/mol	Joback Method
hfus	19.54	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.556		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1545.40		NIST Webbook
rinpol	1545.40		NIST Webbook
tb	603.43	K	Joback Method
tc	813.54	K	Joback Method
tf	354.29	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.05	J/mol×K	603.43	Joback Method
cpg	410.07	J/mol×K	638.45	Joback Method
cpg	423.37	J/mol×K	673.47	Joback Method
cpg	435.94	J/mol×K	708.49	Joback Method
cpg	447.77	J/mol×K	743.51	Joback Method
cpg	458.83	J/mol×K	778.52	Joback Method
cpg	469.13	J/mol×K	813.54	Joback Method

dvisc	0.0011933	Pa×s	354.29	Joback Method
dvisc	0.0006642	Pa×s	395.81	Joback Method
dvisc	0.0004132	Pa×s	437.34	Joback Method
dvisc	0.0002791	Pa×s	478.86	Joback Method
dvisc	0.0002007	Pa×s	520.38	Joback Method
dvisc	0.0001516	Pa×s	561.91	Joback Method
dvisc	0.0001189	Pa×s	603.43	Joback Method

Sources

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=U332760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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