Methyl mandelate

Other names:	Methyl dl-mandelate
	Benzeneacetic acid, «alpha»-hydroxy-, methyl ester, (.+/-.)-
	Benzeneacetic acid, «alpha»-hydroxy-, methyl ester, (±)-
	Methyl hydroxy(phenyl)acetate
	DL-Mandelic acid, methyl ester
	NSC 6539
	Methyl 2-hydroxy-2-phenylethanoate
	methyl (±)-glycolate
Inchi:	InChI=1S/C9H10O3/c1-12-9(11)8(10)7-5-3-2-4-6-7/h2-6,8,10H,1H3
InchiKey:	ITATYELQCJRCCK-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COC(=O)C(O)c1ccccc1
Mol. weight [g/mol]:	166.17
CAS:	4358-87-6

Physical Properties

Property code	Value	Unit	Source
gf	-235.87	kJ/mol	Joback Method
hf	-394.87	kJ/mol	Joback Method
hfus	16.46	kJ/mol	Joback Method
hvap	63.35	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	0.893		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	1309.20		NIST Webbook
rinpol	1244.00		NIST Webbook
tb	600.03	K	Joback Method
tc	805.31	K	Joback Method
tf	335.59	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.57	J/mol×K	600.03	Joback Method
cpg	351.39	J/mol×K	771.10	Joback Method
cpg	343.24	J/mol×K	736.89	Joback Method
cpg	334.50	J/mol×K	702.67	Joback Method
cpg	325.16	J/mol×K	668.46	Joback Method
cpg	315.18	J/mol×K	634.24	Joback Method
cpg	358.96	J/mol×K	805.31	Joback Method
dvisc	0.0000761	Pa×s	600.03	Joback Method
dvisc	0.0001179	Pa×s	555.96	Joback Method
dvisc	0.0001971	Pa×s	511.88	Joback Method
dvisc	0.0003629	Pa×s	467.81	Joback Method
dvisc	0.0007586	Pa×s	423.74	Joback Method
dvisc	0.0018822	Pa×s	379.66	Joback Method
dvisc	0.0059290	Pa×s	335.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	1.60	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4358876&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume