Ethyl mandelate

Other names:	Benzeneacetic acid, «alpha»-hydroxy-, ethyl ester
	Mandelic acid, ethyl ester
	Ethyl phenylglycolate
	Mandelsaeureaethylester
	DL-Mandelic acid ethyl ester
	NSC 5307
Inchi:	InChI=1S/C10H12O3/c1-2-13-10(12)9(11)8-6-4-3-5-7-8/h3-7,9,11H,2H2,1H3
InchiKey:	SAXHIDRUJXPDOD-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	CCOC(=O)C(O)c1ccccc1
Mol. weight [g/mol]:	180.20
CAS:	774-40-3

Physical Properties

Property code	Value	Unit	Source
gf	-227.45	kJ/mol	Joback Method
hf	-415.51	kJ/mol	Joback Method
hfus	19.05	kJ/mol	Joback Method
hvap	65.58	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.283		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	622.91	K	Joback Method
tc	825.20	K	Joback Method
tf	346.86	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.77	J/mol×K	622.91	Joback Method
cpg	363.16	J/mol×K	656.63	Joback Method
cpg	373.87	J/mol×K	690.34	Joback Method

cpg	383.91	J/mol×K	724.06	Joback Method
cpg	393.31	J/mol×K	757.77	Joback Method
cpg	402.07	J/mol×K	791.49	Joback Method
cpg	410.23	J/mol×K	825.20	Joback Method
dvisc	0.0050139	Pa×s	346.86	Joback Method
dvisc	0.0015849	Pa×s	392.87	Joback Method
dvisc	0.0006378	Pa×s	438.88	Joback Method
dvisc	0.0003051	Pa×s	484.88	Joback Method
dvisc	0.0001658	Pa×s	530.89	Joback Method
dvisc	0.0000993	Pa×s	576.90	Joback Method
dvisc	0.0000642	Pa×s	622.91	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C774403&Units=SI

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

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