Propanoic acid, 3-hydroxy-, methyl ester

Other names:	Hydracrylic acid, methyl ester
	Methyl «beta»-hydroxypropionate
	Methyl «gamma»-hydroxypropionate
	Methyl hydracrylate
	HOCH2CH2C(O)OCH3
Inchi:	InChI=1S/C4H8O3/c1-7-4(6)2-3-5/h5H,2-3H2,1H3
InchiKey:	RVGLEPQPVDUSOJ-UHFFFAOYSA-N
Formula:	C4H8O3
SMILES:	COC(=O)CCO
Mol. weight [g/mol]:	104.10
CAS:	6149-41-3

Physical Properties

Property code	Value	Unit	Source
gf	-387.94	kJ/mol	Joback Method
hf	-522.92	kJ/mol	Joback Method
hfus	12.99	kJ/mol	Joback Method
hvap	50.33	kJ/mol	Joback Method
log10ws	0.38		Crippen Method
logp	-0.458		Crippen Method
mcvol	80.530	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	453.70	K	NIST Webbook
tc	632.96	K	Joback Method
tf	267.82	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.81	J/mol×K	632.96	Joback Method
cpg	165.79	J/mol×K	459.39	Joback Method
cpg	172.31	J/mol×K	488.32	Joback Method
cpg	178.62	J/mol×K	517.25	Joback Method

cpg	184.73	J/mol×K	546.17	Joback Method
cpg	190.63	J/mol×K	575.10	Joback Method
cpg	196.32	J/mol×K	604.03	Joback Method
dvisc	0.0002191	Pa×s	459.39	Joback Method
dvisc	0.0164842	Pa×s	267.82	Joback Method
dvisc	0.0054671	Pa×s	299.75	Joback Method
dvisc	0.0022425	Pa×s	331.68	Joback Method
dvisc	0.0010757	Pa×s	363.61	Joback Method
dvisc	0.0005809	Pa×s	395.53	Joback Method
dvisc	0.0003440	Pa×s	427.46	Joback Method
hvapt	60.00	kJ/mol	336.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	352.20	K	1.60	NIST Webbook

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=C6149413&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
hvapt: Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume