

Ethyl 3-hydroxy-3-methylbutanoate

Other names:	(CH3)2C(OH)CH2C(O)OC2H5 Butanoic acid, 3-hydroxy-3-methyl-, ethyl ester Ethyl 3-methyl 3-hydroxy-butanoate ethyl 3-hydroxy-3-methylbutyrate
Inchi:	InChI=1S/C7H14O3/c1-4-10-6(8)5-7(2,3)9/h9H,4-5H2,1-3H3
InchiKey:	HKEDUIGHSRRIKD-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	CCOC(=O)CC(C)(C)O
Mol. weight [g/mol]:	146.18
CAS:	18267-36-2

Physical Properties

Property code	Value	Unit	Source
gf	-359.84	kJ/mol	Joback Method
hf	-593.59	kJ/mol	Joback Method
hfus	13.35	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.710		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	929.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	955.00		NIST Webbook
ripol	1407.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1407.00		NIST Webbook
tb	524.80	K	Joback Method
tc	703.84	K	Joback Method
tf	304.05	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.93	J/mol×K	524.80	Joback Method
cpg	302.45	J/mol×K	554.64	Joback Method
cpg	312.47	J/mol×K	584.48	Joback Method
cpg	322.01	J/mol×K	614.32	Joback Method
cpg	331.07	J/mol×K	644.16	Joback Method
cpg	339.68	J/mol×K	674.00	Joback Method
cpg	347.85	J/mol×K	703.84	Joback Method
dvisc	0.0121392	Pa×s	304.05	Joback Method
dvisc	0.0037644	Pa×s	340.84	Joback Method
dvisc	0.0014665	Pa×s	377.63	Joback Method
dvisc	0.0006754	Pa×s	414.42	Joback Method
dvisc	0.0003530	Pa×s	451.22	Joback Method
dvisc	0.0002034	Pa×s	488.01	Joback Method
dvisc	0.0001267	Pa×s	524.80	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=C18267362&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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