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]:	146.19

Physical Properties

Property code	Value	Unit	Source
af	0.6608		Cheméo Relay (1.0)
gf	-359.84	kJ/mol	Joback Method
hf	-720.94	kJ/mol	Cheméo Relay (1.0)
hfus	13.35	kJ/mol	Joback Method
hvap	62.46	kJ/mol	Cheméo Relay (1.0)
ie	9.98	eV	Cheméo Relay (1.0)
log10ws	-0.03		Cheméo Relay (1.0)
logp	0.710		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	930.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	955.00		NIST Webbook
ripol	1407.00		NIST Webbook
ripol	1407.00		NIST Webbook
ripol	1400.00		NIST Webbook
tb	441.90	K	Cheméo Relay (1.0)
tc	636.14	K	Cheméo Relay (1.0)
tf	268.17	K	Cheméo Relay (1.0)
vc	0.465	m3/kmol	Cheméo Relay (1.0)

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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18267362&Units=SI

Legend

af: Acentric Factor
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
ie:	Ionization energy
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