

Butanoic acid, 2-hydroxy-2-methyl-, ethyl ester

Other names:	ethyl 2-hydroxy-2-methylbutanoate ethyl 2-hydroxy-2-methylbutyrate
Inchi:	InChI=1S/C7H14O3/c1-4-7(3,9)6(8)10-5-2/h9H,4-5H2,1-3H3
InchiKey:	KIYWRWLZHQZKKD-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	CCOC(=O)C(C)(O)CC
Mol. weight [g/mol]:	146.18
CAS:	77-70-3

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	910.00		NIST Webbook
rinpol	902.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1303.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1301.00		NIST Webbook
tb	524.80	K	Joback Method
tc	703.84	K	Joback Method
tf	304.05	K	Joback Method
vc	0.460	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	291.93	J/molxK	524.80	Joback Method
cpg	302.45	J/molxK	554.64	Joback Method
cpg	312.47	J/molxK	584.48	Joback Method
cpg	322.01	J/molxK	614.32	Joback Method
cpg	331.07	J/molxK	644.16	Joback Method
cpg	339.68	J/molxK	674.00	Joback Method
cpg	347.85	J/molxK	703.84	Joback Method
dvisc	0.0121392	Paxs	304.05	Joback Method
dvisc	0.0037644	Paxs	340.84	Joback Method
dvisc	0.0014665	Paxs	377.63	Joback Method
dvisc	0.0006754	Paxs	414.42	Joback Method
dvisc	0.0003530	Paxs	451.22	Joback Method
dvisc	0.0002034	Paxs	488.01	Joback Method
dvisc	0.0001267	Paxs	524.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77703&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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