

Ethyl 2-hydroxy-3,3-dimethylbutyrate

Inchi:	InChI=1S/C8H16O3/c1-5-11-7(10)6(9)8(2,3)4/h6,9H,5H2,1-4H3
InchiKey:	LNSCMKSSQGPHCU-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CCOC(=O)C(O)C(C)(C)C
Mol. weight [g/mol]:	160.21

Physical Properties

Property code	Value	Unit	Source
gf	-353.86	kJ/mol	Joback Method
hf	-619.51	kJ/mol	Joback Method
hfus	12.41	kJ/mol	Joback Method
hvap	57.55	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.956		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	1050.00		NIST Webbook
rinpol	1050.00		NIST Webbook
ripol	1469.00		NIST Webbook
tb	547.24	K	Joback Method
tc	728.02	K	Joback Method
tf	300.32	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.14	J/molxK	547.24	Joback Method
cpg	389.92	J/molxK	697.89	Joback Method
cpg	380.43	J/molxK	667.76	Joback Method
cpg	370.42	J/molxK	637.63	Joback Method
cpg	359.89	J/molxK	607.50	Joback Method
cpg	348.80	J/molxK	577.37	Joback Method
cpg	398.91	J/molxK	728.02	Joback Method

dvisc	0.0000979	Paxs	547.24	Joback Method
dvisc	0.0001629	Paxs	506.09	Joback Method
dvisc	0.0002969	Paxs	464.93	Joback Method
dvisc	0.0006077	Paxs	423.78	Joback Method
dvisc	0.0014513	Paxs	382.63	Joback Method
dvisc	0.0042752	Paxs	341.47	Joback Method
dvisc	0.0169327	Paxs	300.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R420574&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
mvol:	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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