BUTANOIC ACID, 3-HYDROXY-2,2-DIMETHYL-, ETHYL ESTER

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

Physical Properties

Property code	Value	Unit	Source
af	0.5876		Cheméo Relay (1.0)
hf	-714.65	kJ/mol	Cheméo Relay (1.0)
hfus	12.41	kJ/mol	Joback Method
hvap	65.64	kJ/mol	Cheméo Relay (1.0)
ie	9.93	eV	Cheméo Relay (1.0)
logp	0.956		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
ripol	1699.00		NIST Webbook
ripol	1699.00		NIST Webbook
tb	454.68	K	Cheméo Relay (1.0)
tc	652.42	K	Cheméo Relay (1.0)
tf	275.08	K	Cheméo Relay (1.0)
vc	0.497	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

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

Sources

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=C7505944&Units=SI
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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume