Butanoic acid, 2,3-dimethyl-, ethyl ester

Other names: Ethyl 2,3-dimethylbutanoate
Inchi: InChI=1S/C8H16O2/c1-5-10-8(9)7(4)6(2)3/h6-7H,5H2,1-4H3
InchiKey: UOLDHHQOKRYISV-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCOC(=O)C(C)C(C)C
Mol. weight [g/mol]: 144.21
CAS: 54004-42-1

Physical Properties

Property code	Value	Unit	Source
gf	-222.32	kJ/mol	Joback Method
hf	-463.81	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	41.78	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.842		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	908.00		NIST Webbook
tb	457.85	K	Joback Method
tc	640.65	K	Joback Method
tf	222.08	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.95	J/mol×K	457.85	Joback Method
cpg	292.89	J/mol×K	488.32	Joback Method
cpg	305.35	J/mol×K	518.78	Joback Method
cpg	317.32	J/mol×K	549.25	Joback Method
cpg	328.83	J/mol×K	579.72	Joback Method
cpg	339.86	J/mol×K	610.19	Joback Method
cpg	350.42	J/mol×K	640.65	Joback Method

dvisc	0.0076048	Pa×s	222.08	Joback Method
dvisc	0.0027406	Pa×s	261.38	Joback Method
dvisc	0.0012896	Pa×s	300.67	Joback Method
dvisc	0.0007223	Pa×s	339.97	Joback Method
dvisc	0.0004562	Pa×s	379.26	Joback Method
dvisc	0.0003141	Pa×s	418.56	Joback Method
dvisc	0.0002306	Pa×s	457.85	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C54004421&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume