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

Other names: Butyric acid, 2,3-dimethyl-, methyl ester
Inchi: InChI=1S/C7H14O2/c1-5(2)6(3)7(8)9-4/h5-6H,1-4H3
InchiKey: YLXGEYQXFJAIBQ-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: COC(=O)C(C)C(C)C
Mol. weight [g/mol]: 130.18
CAS: 30540-29-5

Physical Properties

Property code	Value	Unit	Source
gf	-230.74	kJ/mol	Joback Method
hf	-443.17	kJ/mol	Joback Method
hfus	9.63	kJ/mol	Joback Method
hvap	39.56	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.451		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	763.00		NIST Webbook
tb	434.97	K	Joback Method
tc	619.42	K	Joback Method
tf	210.81	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.81	J/mol×K	434.97	Joback Method
cpg	250.59	J/mol×K	465.71	Joback Method
cpg	261.96	J/mol×K	496.45	Joback Method
cpg	272.90	J/mol×K	527.19	Joback Method
cpg	283.42	J/mol×K	557.94	Joback Method
cpg	293.53	J/mol×K	588.68	Joback Method
cpg	303.21	J/mol×K	619.42	Joback Method

dvisc	0.0077039	Pa×s	210.81	Joback Method
dvisc	0.0028076	Pa×s	248.17	Joback Method
dvisc	0.0013326	Pa×s	285.53	Joback Method
dvisc	0.0007515	Pa×s	322.89	Joback Method
dvisc	0.0004773	Pa×s	360.25	Joback Method
dvisc	0.0003301	Pa×s	397.61	Joback Method
dvisc	0.0002432	Pa×s	434.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30540295&Units=SI
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

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