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

Other names:	Butyric acid, 2,2-dimethyl-, methyl ester
	Methyl «alpha»,«alpha»-dimethylbutyrate
	Methyl 2,2-dimethylbutyrate
Inchi:	InChI=1S/C7H14O2/c1-5-7(2,3)6(8)9-4/h5H2,1-4H3
InchiKey:	IGHXQNDUQCTKSH-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCC(C)(C)C(=O)OC
Mol. weight [g/mol]:	130.18
CAS:	813-67-2

Physical Properties

Property code	Value	Unit	Source
gf	-223.02	kJ/mol	Joback Method
hf	-441.36	kJ/mol	Joback Method
hfus	9.26	kJ/mol	Joback Method
hvap	39.04	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	845.00		NIST Webbook
rinpol	845.00		NIST Webbook
tb	432.62	K	Joback Method
tc	620.42	K	Joback Method
tf	243.23	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.05	J/mol×K	432.62	Joback Method
cpg	253.38	J/mol×K	463.92	Joback Method
cpg	265.15	J/mol×K	495.22	Joback Method
cpg	276.37	J/mol×K	526.52	Joback Method

cpg	287.06	J/mol×K	557.82	Joback Method
cpg	297.22	J/mol×K	589.12	Joback Method
cpg	306.89	J/mol×K	620.42	Joback Method
dvisc	0.0047587	Pa×s	243.23	Joback Method
dvisc	0.0022582	Pa×s	274.80	Joback Method
dvisc	0.0012495	Pa×s	306.36	Joback Method
dvisc	0.0007722	Pa×s	337.93	Joback Method
dvisc	0.0005181	Pa×s	369.49	Joback Method
dvisc	0.0003702	Pa×s	401.06	Joback Method
dvisc	0.0002778	Pa×s	432.62	Joback Method

Sources

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=C813672&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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