Butanoic acid, 3,3-dimethyl-2-(1-methylethyl), ethyl ester

Other names: Butanoic acid, 2-isopropyl-3,3-dimethyl, ethyl ester
Inchi: InChI=1S/C11H22O2/c1-7-13-10(12)9(8(2)3)11(4,5)6/h8-9H,7H2,1-6H3
InchiKey: RSBMHLDDEJRKMZ-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: CCOC(=O)C(C(C)C)C(C)(C)C
Mol. weight [g/mol]: 186.29

Physical Properties

Property code	Value	Unit	Source
gf	-194.22	kJ/mol	Joback Method
hf	-534.48	kJ/mol	Joback Method
hfus	12.57	kJ/mol	Joback Method
hvap	47.16	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.868		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1102.00		NIST Webbook
rinpol	1102.00		NIST Webbook
tb	523.26	K	Joback Method
tc	711.19	K	Joback Method
tf	258.31	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.60	J/mol×K	523.26	Joback Method
cpg	435.34	J/mol×K	554.58	Joback Method
cpg	451.26	J/mol×K	585.90	Joback Method
cpg	466.40	J/mol×K	617.23	Joback Method
cpg	480.77	J/mol×K	648.55	Joback Method
cpg	494.41	J/mol×K	679.87	Joback Method
cpg	507.33	J/mol×K	711.19	Joback Method

dvisc	0.0092666	Pa×s	258.31	Joback Method
dvisc	0.0029409	Pa×s	302.47	Joback Method
dvisc	0.0012504	Pa×s	346.63	Joback Method
dvisc	0.0006450	Pa×s	390.78	Joback Method
dvisc	0.0003806	Pa×s	434.94	Joback Method
dvisc	0.0002475	Pa×s	479.10	Joback Method
dvisc	0.0001731	Pa×s	523.26	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=R108264&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