Butanoic acid, 2-isopropyl-2,3,3-trimethyl, ethyl ester

Other names: Butanoic acid, 2,3,3-trimethyl-2-(1-methylethyl), ethyl ester
Inchi: InChI=1S/C12H24O2/c1-8-14-10(13)12(7,9(2)3)11(4,5)6/h9H,8H2,1-7H3
InchiKey: AYKXSKJFLXRXGM-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CCOC(=O)C(C)(C(C)C)C(C)(C)C
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
gf	-180.52	kJ/mol	Joback Method
hf	-558.59	kJ/mol	Joback Method
hfus	11.27	kJ/mol	Joback Method
hvap	48.48	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	3.258		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1237.00		NIST Webbook
tb	543.35	K	Joback Method
tc	736.01	K	Joback Method
tf	287.00	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.19	J/mol×K	543.35	Joback Method
cpg	488.23	J/mol×K	575.46	Joback Method
cpg	505.28	J/mol×K	607.57	Joback Method
cpg	521.37	J/mol×K	639.68	Joback Method
cpg	536.56	J/mol×K	671.79	Joback Method
cpg	550.88	J/mol×K	703.90	Joback Method
cpg	564.37	J/mol×K	736.01	Joback Method
dvisc	0.0070187	Pa×s	287.00	Joback Method

dvisc	0.0024540	Pa×s	329.73	Joback Method
dvisc	0.0010919	Pa×s	372.45	Joback Method
dvisc	0.0005740	Pa×s	415.18	Joback Method
dvisc	0.0003402	Pa×s	457.90	Joback Method
dvisc	0.0002205	Pa×s	500.62	Joback Method
dvisc	0.0001530	Pa×s	543.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R108195&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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