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

Other names: Butanoic acid, 3-methyl-2-(1-methylethyl), ethyl ester
Inchi: InChI=1S/C10H20O2/c1-6-12-10(11)9(7(2)3)8(4)5/h7-9H,6H2,1-5H3
InchiKey: GNBAFGHDBAZUPW-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CCOC(=O)C(C(C)C)C(C)C
Mol. weight [g/mol]: 172.26

Physical Properties

Property code	Value	Unit	Source
gf	-207.92	kJ/mol	Joback Method
hf	-510.37	kJ/mol	Joback Method
hfus	13.87	kJ/mol	Joback Method
hvap	45.85	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.478		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
tb	503.17	K	Joback Method
tc	686.24	K	Joback Method
tf	229.62	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.71	J/mol×K	503.17	Joback Method
cpg	438.85	J/mol×K	655.73	Joback Method
cpg	426.03	J/mol×K	625.22	Joback Method
cpg	412.61	J/mol×K	594.71	Joback Method
cpg	398.59	J/mol×K	564.19	Joback Method
cpg	383.96	J/mol×K	533.68	Joback Method
cpg	451.08	J/mol×K	686.24	Joback Method

dvisc	0.0001885	Pa×s	503.17	Joback Method
dvisc	0.0002658	Pa×s	457.58	Joback Method
dvisc	0.0004042	Pa×s	411.99	Joback Method
dvisc	0.0006824	Pa×s	366.39	Joback Method
dvisc	0.0013368	Pa×s	320.80	Joback Method
dvisc	0.0032727	Pa×s	275.21	Joback Method
dvisc	0.0114324	Pa×s	229.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R108279&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