Butanoic acid, 2-methyl-, 1-methylpropyl ester

Other names: Butyric acid, 2-methyl-, sec-butyl ester
Inchi: InChI=1S/C9H18O2/c1-5-7(3)9(10)11-8(4)6-2/h7-8H,5-6H2,1-4H3
InchiKey: DENXFTQQZIKUAY-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCC(C)OC(=O)C(C)CC
Mol. weight [g/mol]: 158.24
CAS: 869-08-9

Physical Properties

Property code	Value	Unit	Source
gf	-213.90	kJ/mol	Joback Method
hf	-484.45	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	44.01	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.374		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	971.00		NIST Webbook
ripol	1148.00		NIST Webbook
tb	480.73	K	Joback Method
tc	661.81	K	Joback Method
tf	233.35	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.22	J/mol×K	480.73	Joback Method
cpg	337.19	J/mol×K	510.91	Joback Method
cpg	350.61	J/mol×K	541.09	Joback Method
cpg	363.51	J/mol×K	571.27	Joback Method
cpg	375.88	J/mol×K	601.45	Joback Method
cpg	387.73	J/mol×K	631.63	Joback Method

cpg	399.06	J/mol×K	661.81	Joback Method
dvisc	0.0073761	Pa×s	233.35	Joback Method
dvisc	0.0026314	Pa×s	274.58	Joback Method
dvisc	0.0012286	Pa×s	315.81	Joback Method
dvisc	0.0006840	Pa×s	357.04	Joback Method
dvisc	0.0004299	Pa×s	398.27	Joback Method
dvisc	0.0002948	Pa×s	439.50	Joback Method
dvisc	0.0002156	Pa×s	480.73	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=C869089&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume