butanoic acid, 1,2-dimethylpropyl ester

Inchi: InChI=1S/C9H18O2/c1-5-6-9(10)11-8(4)7(2)3/h7-8H,5-6H2,1-4H3
InchiKey: YBSMWGNIGFSKPE-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 158.24
CAS: 88736-68-9

Physical Properties

Property code	Value	Unit	Source
af	0.5020		Cheméo Relay (1.0)
hf	-572.71	kJ/mol	Cheméo Relay (1.0)
hfus	14.81	kJ/mol	Joback Method
hvap	49.32	kJ/mol	Cheméo Relay (1.0)
ie	9.85	eV	Cheméo Relay (1.0)
log10ws	-2.24		Cheméo Relay (1.0)
logp	2.374		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
tb	425.65	K	Cheméo Relay (1.0)
tc	607.91	K	Cheméo Relay (1.0)
tf	192.70	K	Cheméo Relay (1.0)
vc	0.536	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88736689&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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