Propanoic acid, 2,2-dimethyl, 1-methylpropyl ester

Inchi: InChI=1S/C9H18O2/c1-6-7(2)11-8(10)9(3,4)5/h7H,6H2,1-5H3
InchiKey: DTXXVVZDBVWESG-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCC(C)OC(=O)C(C)(C)C
Mol. weight [g/mol]: 158.24

Physical Properties

Property code	Value	Unit	Source
gf	-208.62	kJ/mol	Joback Method
hf	-487.92	kJ/mol	Joback Method
hfus	10.92	kJ/mol	Joback Method
hvap	43.10	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.374		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	904.00		NIST Webbook
rinpol	904.00		NIST Webbook
ripol	1044.00		NIST Webbook
tb	477.94	K	Joback Method
tc	666.16	K	Joback Method
tf	250.77	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.82	J/mol×K	477.94	Joback Method
cpg	392.85	J/mol×K	634.79	Joback Method
cpg	380.76	J/mol×K	603.42	Joback Method
cpg	368.03	J/mol×K	572.05	Joback Method
cpg	354.64	J/mol×K	540.68	Joback Method
cpg	340.58	J/mol×K	509.31	Joback Method
cpg	404.33	J/mol×K	666.16	Joback Method

dvisc	0.0002253	Pa×s	477.94	Joback Method
dvisc	0.0003117	Pa×s	440.08	Joback Method
dvisc	0.0004585	Pa×s	402.22	Joback Method
dvisc	0.0007309	Pa×s	364.36	Joback Method
dvisc	0.0012980	Pa×s	326.49	Joback Method
dvisc	0.0026801	Pa×s	288.63	Joback Method
dvisc	0.0068881	Pa×s	250.77	Joback Method

Sources

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=R10557&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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