Octanoic acid, 2,2-dimethyl, methyl ester

Other names: methyl 2,2-dimethyloctanoate
Inchi: InChI=1S/C11H22O2/c1-5-6-7-8-9-11(2,3)10(12)13-4/h5-9H2,1-4H3
InchiKey: BAKOMPNQDRRCQN-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: CCCCCCC(C)(C)C(=O)OC
Mol. weight [g/mol]: 186.29
CAS: 14250-74-9

Physical Properties

Property code	Value	Unit	Source
gf	-189.34	kJ/mol	Joback Method
hf	-523.92	kJ/mol	Joback Method
hfus	19.62	kJ/mol	Joback Method
hvap	47.94	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.156		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1128.00		NIST Webbook
rinpol	1128.00		NIST Webbook
tb	524.14	K	Joback Method
tc	704.63	K	Joback Method
tf	288.31	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.15	J/mol×K	524.14	Joback Method
cpg	434.09	J/mol×K	554.22	Joback Method
cpg	449.29	J/mol×K	584.30	Joback Method
cpg	463.79	J/mol×K	614.38	Joback Method
cpg	477.60	J/mol×K	644.47	Joback Method
cpg	490.74	J/mol×K	674.55	Joback Method

cpg	503.23	J/mol×K	704.63	Joback Method
dvisc	0.0041126	Pa×s	288.31	Joback Method
dvisc	0.0018231	Pa×s	327.62	Joback Method
dvisc	0.0009620	Pa×s	366.92	Joback Method
dvisc	0.0005745	Pa×s	406.23	Joback Method
dvisc	0.0003757	Pa×s	445.53	Joback Method
dvisc	0.0002633	Pa×s	484.84	Joback Method
dvisc	0.0001946	Pa×s	524.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14250749&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

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