Tetradecanoic acid, 10,13-dimethyl-, methyl ester

Inchi: InChI=1S/C17H34O2/c1-15(2)13-14-16(3)11-9-7-5-6-8-10-12-17(18)19-4/h15-16H,5-14H
InchiKey: YMXLTDXXQGMDPS-UHFFFAOYSA-N
Formula: C17H34O2
SMILES: COC(=O)CCCCCCCCC(C)CCC(C)C
Mol. weight [g/mol]: 270.45
CAS: 267650-23-7

Physical Properties

Property code	Value	Unit	Source
gf	-146.54	kJ/mol	Joback Method
hf	-649.57	kJ/mol	Joback Method
hfus	35.53	kJ/mol	Joback Method
hvap	61.82	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.353		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	1926.00		NIST Webbook
tb	663.77	K	Joback Method
tc	835.50	K	Joback Method
tf	323.51	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.07	J/mol×K	663.77	Joback Method
cpg	751.93	J/mol×K	692.39	Joback Method
cpg	769.95	J/mol×K	721.01	Joback Method
cpg	787.14	J/mol×K	749.64	Joback Method
cpg	803.52	J/mol×K	778.26	Joback Method
cpg	819.11	J/mol×K	806.88	Joback Method
cpg	833.92	J/mol×K	835.50	Joback Method
dvisc	0.0038870	Pa×s	323.51	Joback Method

dvisc	0.0013124	Pa×s	380.22	Joback Method
dvisc	0.0005874	Pa×s	436.93	Joback Method
dvisc	0.0003162	Pa×s	493.64	Joback Method
dvisc	0.0001934	Pa×s	550.35	Joback Method
dvisc	0.0001297	Pa×s	607.06	Joback Method
dvisc	0.0000931	Pa×s	663.77	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C267650237&Units=SI

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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