Tetradecanoic acid, 12-methyl-, methyl ester

Other names: Methyl 12-methyltetradecanoate
Methyl tetradecanoate, 12-methyl
Inchi: InChI=1S/C16H32O2/c1-4-15(2)13-11-9-7-5-6-8-10-12-14-16(17)18-3/h15H,4-14H2,1-3H
InchiKey: BJIUDNXPLSJWKE-UHFFFAOYSA-N
Formula: C16H32O2
SMILES: CCC(C)CCCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 256.42
CAS: 5129-66-8

Physical Properties

Property code	Value	Unit	Source
gf	-152.52	kJ/mol	Joback Method
hf	-623.65	kJ/mol	Joback Method
hfus	36.46	kJ/mol	Joback Method
hvap	59.98	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	5.107		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1786.00		NIST Webbook
rinpol	1786.00		NIST Webbook
rinpol	1771.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1786.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	641.33	K	Joback Method
tc	810.93	K	Joback Method
tf	327.24	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.23	J/mol×K	641.33	Joback Method
cpg	694.40	J/mol×K	669.60	Joback Method
cpg	711.78	J/mol×K	697.86	Joback Method
cpg	728.40	J/mol×K	726.13	Joback Method
cpg	744.26	J/mol×K	754.40	Joback Method
cpg	759.39	J/mol×K	782.67	Joback Method
cpg	773.80	J/mol×K	810.93	Joback Method
dvisc	0.0031617	Pa×s	327.24	Joback Method
dvisc	0.0012389	Pa×s	379.59	Joback Method
dvisc	0.0006092	Pa×s	431.94	Joback Method
dvisc	0.0003493	Pa×s	484.28	Joback Method
dvisc	0.0002232	Pa×s	536.63	Joback Method
dvisc	0.0001544	Pa×s	588.98	Joback Method
dvisc	0.0001135	Pa×s	641.33	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=C5129668&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
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume