Pentadecanoic acid, 14-methyl-, methyl ester

Other names: Methyl isohexadecanoate
Inchi: InChI=1S/C17H34O2/c1-16(2)14-12-10-8-6-4-5-7-9-11-13-15-17(18)19-3/h16H,4-15H2,1
InchiKey: WAKCWJNDXBPEBP-UHFFFAOYSA-N
Formula: C17H34O2
SMILES: COC(=O)CCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 270.45
CAS: 5129-60-2

Physical Properties

Property code	Value	Unit	Source
gf	-144.10	kJ/mol	Joback Method
hf	-644.29	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.497		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	1877.00		NIST Webbook
rinpol	1877.00		NIST Webbook
rinpol	1887.00		NIST Webbook
rinpol	1861.00		NIST Webbook
rinpol	1884.00		NIST Webbook
ripol	2166.00		NIST Webbook
tb	664.21	K	Joback Method
tc	833.82	K	Joback Method
tf	338.51	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.67	J/mol×K	664.21	Joback Method
cpg	751.27	J/mol×K	692.48	Joback Method

cpg	769.05	J/mol×K	720.75	Joback Method
cpg	786.03	J/mol×K	749.02	Joback Method
cpg	802.22	J/mol×K	777.28	Joback Method
cpg	817.65	J/mol×K	805.55	Joback Method
cpg	832.34	J/mol×K	833.82	Joback Method
dvisc	0.0028787	Pa×s	338.51	Joback Method
dvisc	0.0011177	Pa×s	392.79	Joback Method
dvisc	0.0005461	Pa×s	447.08	Joback Method
dvisc	0.0003116	Pa×s	501.36	Joback Method
dvisc	0.0001983	Pa×s	555.64	Joback Method
dvisc	0.0001368	Pa×s	609.93	Joback Method
dvisc	0.0001003	Pa×s	664.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5129602&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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