Hexadecanoic acid, 15-methyl-, methyl ester

Other names: Methyl isoheptadecanoate
Methyl 15-methylhexadecanoate
Inchi: InChI=1S/C18H36O2/c1-17(2)15-13-11-9-7-5-4-6-8-10-12-14-16-18(19)20-3/h17H,4-16H
InchiKey: BNHKXOIJKIMOJH-UHFFFAOYSA-N
Formula: C18H36O2
SMILES: COC(=O)CCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 284.48
CAS: 6929-04-0

Physical Properties

Property code	Value	Unit	Source
gf	-135.68	kJ/mol	Joback Method
hf	-664.93	kJ/mol	Joback Method
hfus	41.64	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.887		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	1974.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
tb	687.09	K	Joback Method
tc	857.14	K	Joback Method
tf	349.78	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.33	J/mol×K	687.09	Joback Method

cpg	809.34	J/mol×K	715.43	Joback Method
cpg	827.49	J/mol×K	743.77	Joback Method
cpg	844.81	J/mol×K	772.12	Joback Method
cpg	861.31	J/mol×K	800.46	Joback Method
cpg	877.02	J/mol×K	828.80	Joback Method
cpg	891.94	J/mol×K	857.14	Joback Method
dvisc	0.0026053	Pa×s	349.78	Joback Method
dvisc	0.0010029	Pa×s	406.00	Joback Method
dvisc	0.0004870	Pa×s	462.22	Joback Method
dvisc	0.0002766	Pa×s	518.43	Joback Method
dvisc	0.0001755	Pa×s	574.65	Joback Method
dvisc	0.0001207	Pa×s	630.87	Joback Method
dvisc	0.0000883	Pa×s	687.09	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=C6929040&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