

Hexadecanoic acid, 2-hydroxy-14-methyl, methyl ester

Inchi:	InChI=1S/C18H36O3/c1-4-16(2)14-12-10-8-6-5-7-9-11-13-15-17(19)18(20)21-3/h16-17,1
InchiKey:	KKKGECOONXFWRE-UHFFFAOYSA-N
Formula:	C18H36O3
SMILES:	CCC(C)CCCCCCCCCCC(O)C(=O)OC
Mol. weight [g/mol]:	300.48

Physical Properties

Property code	Value	Unit	Source
gf	-274.94	kJ/mol	Joback Method
hf	-822.44	kJ/mol	Joback Method
hfus	42.20	kJ/mol	Joback Method
hvap	80.72	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.858		Crippen Method
mcvol	277.790	ml/mol	McGowan Method
pc	1282.83	kPa	Joback Method
rinpol	2102.00		NIST Webbook
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tb	778.83	K	Joback Method
tc	956.64	K	Joback Method
tf	395.60	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.49	J/molxK	778.83	Joback Method
cpg	884.65	J/molxK	808.46	Joback Method
cpg	900.92	J/molxK	838.10	Joback Method
cpg	916.33	J/molxK	867.73	Joback Method
cpg	930.91	J/molxK	897.37	Joback Method
cpg	944.67	J/molxK	927.00	Joback Method
cpg	957.64	J/molxK	956.64	Joback Method
dvisc	0.0026782	Paxs	395.60	Joback Method

dvisc	0.0006189	Paxs	459.47	Joback Method
dvisc	0.0002045	Paxs	523.34	Joback Method
dvisc	0.0000860	Paxs	587.22	Joback Method
dvisc	0.0000429	Paxs	651.09	Joback Method
dvisc	0.0000242	Paxs	714.96	Joback Method
dvisc	0.0000150	Paxs	778.83	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=R98113&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

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