Methyl 2-hydroxy-heptadecanoate

Other names: Heptadecanoic acid, 2-hydroxy, methyl ester
Inchi: InChI=1S/C18H36O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(19)18(20)21-2/h17,19H
InchiKey: OGSBNYHFFMLFJI-UHFFFAOYSA-N
Formula: C18H36O3
SMILES: CCCCCCCCCCCCCCCC(O)C(=O)OC
Mol. weight [g/mol]: 300.48

Physical Properties

Property code	Value	Unit	Source
gf	-272.50	kJ/mol	Joback Method
hf	-817.16	kJ/mol	Joback Method
hfus	45.73	kJ/mol	Joback Method
hvap	81.11	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.002		Crippen Method
mcvol	277.790	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook
tb	779.27	K	Joback Method
tc	956.35	K	Joback Method
tf	410.60	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.00	J/mol×K	779.27	Joback Method
cpg	884.08	J/mol×K	808.78	Joback Method
cpg	900.29	J/mol×K	838.30	Joback Method
cpg	915.65	J/mol×K	867.81	Joback Method
cpg	930.20	J/mol×K	897.33	Joback Method
cpg	943.94	J/mol×K	926.84	Joback Method
cpg	956.90	J/mol×K	956.35	Joback Method

dvisc	0.0019004	Pa×s	410.60	Joback Method
dvisc	0.0005130	Pa×s	472.05	Joback Method
dvisc	0.0001872	Pa×s	533.49	Joback Method
dvisc	0.0000841	Pa×s	594.93	Joback Method
dvisc	0.0000439	Pa×s	656.38	Joback Method
dvisc	0.0000256	Pa×s	717.83	Joback Method
dvisc	0.0000163	Pa×s	779.27	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=U336201&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