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

Inchi: InChI=1S/C18H36O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-18(2,20)17(19)21-3/h20H,4-1

InchiKey: LJDOGPABVJTNTI-UHFFFAOYSA-N

Formula: C18H36O3

SMILES: CCCCCCCCCCCCCCC(C)(O)C(=O)OC

Mol. weight [g/mol]: 300.48

Physical Properties

Property code	Value	Unit	Source
gf	-267.22	kJ/mol	Joback Method
hf	-820.63	kJ/mol	Joback Method
hfus	41.84	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.002		Crippen Method
mcvol	277.790	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	776.48	K	Joback Method
tc	954.68	K	Joback Method
tf	428.02	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.90	J/mol×K	776.48	Joback Method
cpg	884.85	J/mol×K	806.18	Joback Method
cpg	900.93	J/mol×K	835.88	Joback Method
cpg	916.17	J/mol×K	865.58	Joback Method
cpg	930.60	J/mol×K	895.28	Joback Method
cpg	944.27	J/mol×K	924.98	Joback Method
cpg	957.21	J/mol×K	954.68	Joback Method
dvisc	0.0013583	Pa×s	428.02	Joback Method

dvisc	0.0004052	Pa×s	486.10	Joback Method
dvisc	0.0001565	Pa×s	544.17	Joback Method
dvisc	0.0000726	Pa×s	602.25	Joback Method
dvisc	0.0000385	Pa×s	660.33	Joback Method
dvisc	0.0000227	Pa×s	718.40	Joback Method
dvisc	0.0000144	Pa×s	776.48	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=R98131&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