Hexadecanoic acid, 11-hydroxy-, methyl ester

Other names:	Methyl 11-hydroxyhexadecanoate
	11-Hydroxyhexadecanoic acid, methyl ester
	Methyl jalapinolate
	Jalapinolic acid, methyl ester
Inchi:	InChI=1S/C17H34O3/c1-3-4-10-13-16(18)14-11-8-6-5-7-9-12-15-17(19)20-2/h16,18H,3-1
InchiKey:	HVZSXWZMSOPRCP-UHFFFAOYSA-N
Formula:	C17H34O3
SMILES:	CCCCCC(O)CCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	286.45
CAS:	60368-18-5

Physical Properties

Property code	Value	Unit	Source
gf	-280.92	kJ/mol	Joback Method
hf	-796.52	kJ/mol	Joback Method
hfus	43.14	kJ/mol	Joback Method
hvap	78.88	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.612		Crippen Method
mcvol	263.700	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
tb	756.39	K	Joback Method
tc	930.60	K	Joback Method
tf	399.33	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.17	J/mol×K	756.39	Joback Method
cpg	882.98	J/mol×K	901.56	Joback Method
cpg	869.56	J/mol×K	872.53	Joback Method
cpg	855.40	J/mol×K	843.49	Joback Method
cpg	840.45	J/mol×K	814.46	Joback Method

cpg	824.72	J/mol×K	785.42	Joback Method
cpg	895.65	J/mol×K	930.60	Joback Method
dvisc	0.0000196	Pa×s	756.39	Joback Method
dvisc	0.0000310	Pa×s	696.88	Joback Method
dvisc	0.0000532	Pa×s	637.37	Joback Method
dvisc	0.0001021	Pa×s	577.86	Joback Method
dvisc	0.0002277	Pa×s	518.35	Joback Method
dvisc	0.0006252	Pa×s	458.84	Joback Method
dvisc	0.0023196	Pa×s	399.33	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60368185&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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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