Hexadecanoic acid, 2-hydroxy-, methyl ester

Inchi: InChI=1S/C17H34O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16(18)17(19)20-2/h16,18H,3-1
InchiKey: LQZITXGTIYKQBJ-UHFFFAOYSA-N
Formula: C17H34O3
SMILES: CCCCCCCCCCCCCCC(O)C(=O)OC
Mol. weight [g/mol]: 286.45
CAS: 16742-51-1

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
rinpol	2046.80		NIST Webbook
rinpol	2048.00		NIST Webbook
rinpol	2048.00		NIST Webbook
rinpol	2046.80		NIST Webbook
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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16742511&Units=SI

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