Octadecanoic acid, 9,10-dihydroxy-, methyl ester

Other names: Methyl 9,10-dihydroxystearate
methyl 9,10-dihydroxyoctadecanoate
Inchi: InChI=1S/C19H38O4/c1-3-4-5-6-8-11-14-17(20)18(21)15-12-9-7-10-13-16-19(22)23-2/h1
InchiKey: RITHLQKJQSKUAO-UHFFFAOYSA-N
Formula: C19H38O4
SMILES: CCCCCCCCC(O)C(O)CCCCCCCC(=O)OC
Mol. weight [g/mol]: 330.50
CAS: 1115-01-1

Physical Properties

Property code	Value	Unit	Source
gf	-403.34	kJ/mol	Joback Method
hf	-995.31	kJ/mol	Joback Method
hfus	48.88	kJ/mol	Joback Method
hvap	99.63	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.363		Crippen Method
mcvol	297.750	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook
tb	893.89	K	Joback Method
tc	1097.23	K	Joback Method
tf	467.69	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.66	J/mol×K	893.89	Joback Method
cpg	1013.40	J/mol×K	927.78	Joback Method
cpg	1029.05	J/mol×K	961.67	Joback Method
cpg	1043.66	J/mol×K	995.56	Joback Method
cpg	1057.25	J/mol×K	1029.45	Joback Method

cpg	1069.86	J/mol×K	1063.34	Joback Method
cpg	1081.55	J/mol×K	1097.23	Joback Method
dvisc	0.0006691	Pa×s	467.69	Joback Method
dvisc	0.0001239	Pa×s	538.72	Joback Method
dvisc	0.0000340	Pa×s	609.76	Joback Method
dvisc	0.0000122	Pa×s	680.79	Joback Method
dvisc	0.0000053	Pa×s	751.82	Joback Method
dvisc	0.0000027	Pa×s	822.86	Joback Method
dvisc	0.0000015	Pa×s	893.89	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1115011&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume