Octadecanoic acid, 17-methyl-, methyl ester

Inchi: InChI=1S/C20H40O2/c1-19(2)17-15-13-11-9-7-5-4-6-8-10-12-14-16-18-20(21)22-3/h19H
InchiKey: MASZVQKLIMRPFY-UHFFFAOYSA-N
Formula: C20H40O2
SMILES: COC(=O)CCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 312.53
CAS: 55124-97-5

Physical Properties

Property code	Value	Unit	Source
gf	-118.84	kJ/mol	Joback Method
hf	-706.21	kJ/mol	Joback Method
hfus	46.82	kJ/mol	Joback Method
hvap	68.88	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	6.667		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
tb	732.85	K	Joback Method
tc	905.32	K	Joback Method
tf	372.32	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.95	J/mol×K	732.85	Joback Method
cpg	928.77	J/mol×K	761.59	Joback Method
cpg	947.65	J/mol×K	790.34	Joback Method
cpg	965.61	J/mol×K	819.08	Joback Method
cpg	982.69	J/mol×K	847.83	Joback Method
cpg	998.90	J/mol×K	876.57	Joback Method
cpg	1014.26	J/mol×K	905.32	Joback Method
dvisc	0.0021002	Pa×s	372.32	Joback Method
dvisc	0.0007959	Pa×s	432.41	Joback Method

dvisc	0.0003822	Pa×s	492.50	Joback Method
dvisc	0.0002153	Pa×s	552.59	Joback Method
dvisc	0.0001357	Pa×s	612.67	Joback Method
dvisc	0.0000929	Pa×s	672.76	Joback Method
dvisc	0.0000677	Pa×s	732.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55124975&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