

6,9,12-Octadecatrienoic acid, methyl ester

Inchi:	InChI=1S/C19H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h7-8,10-
InchiKey:	JFRWATCOFCPIBM-SPOHZTNBSA-N
Formula:	C19H32O2
SMILES:	CCCCC=CCC=CC=CCCCC(=O)OC
Mol. weight [g/mol]:	292.46
CAS:	2676-41-7

Physical Properties

Property code	Value	Unit	Source
gf	115.84	kJ/mol	Joback Method
hf	-328.63	kJ/mol	Joback Method
hfus	48.36	kJ/mol	Joback Method
hvap	66.92	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.749		Crippen Method
mcvol	273.110	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
tb	722.89	K	Joback Method
tc	904.64	K	Joback Method
tf	360.81	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.46	J/molxK	722.89	Joback Method
cpg	798.24	J/molxK	753.18	Joback Method
cpg	815.15	J/molxK	783.47	Joback Method
cpg	831.25	J/molxK	813.77	Joback Method
cpg	846.59	J/molxK	844.06	Joback Method
cpg	861.21	J/molxK	874.35	Joback Method
cpg	875.18	J/molxK	904.64	Joback Method
dvisc	0.0015069	Paxs	360.81	Joback Method
dvisc	0.0005818	Paxs	421.16	Joback Method

dvisc	0.0002851	Paxs	481.50	Joback Method
dvisc	0.0001638	Paxs	541.85	Joback Method
dvisc	0.0001052	Paxs	602.20	Joback Method
dvisc	0.0000732	Paxs	662.54	Joback Method
dvisc	0.0000541	Paxs	722.89	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=C2676417&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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