9,12,15-Octadecatrienoic acid, methyl ester

Other names: Methyl 9,12,15-octadecatrienoate
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/h4-5,7-8
InchiKey: DVWSXZIHSUZZKJ-JSIPCRQOSA-N
Formula: C19H32O2
SMILES: CCC=CCC=CCC=CCCCCCCCC(=O)OC
Mol. weight [g/mol]: 292.46
CAS: 7361-80-0

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
rinpol	2085.00		NIST Webbook
rinpol	2086.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2086.00		NIST Webbook
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/mol×K	722.89	Joback Method
cpg	798.24	J/mol×K	753.18	Joback Method
cpg	815.15	J/mol×K	783.47	Joback Method
cpg	831.25	J/mol×K	813.77	Joback Method

cpg	846.59	J/mol×K	844.06	Joback Method
cpg	861.21	J/mol×K	874.35	Joback Method
cpg	875.18	J/mol×K	904.64	Joback Method
dvisc	0.0015069	Pa×s	360.81	Joback Method
dvisc	0.0005818	Pa×s	421.16	Joback Method
dvisc	0.0002851	Pa×s	481.50	Joback Method
dvisc	0.0001638	Pa×s	541.85	Joback Method
dvisc	0.0001052	Pa×s	602.20	Joback Method
dvisc	0.0000732	Pa×s	662.54	Joback Method
dvisc	0.0000541	Pa×s	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=C7361800&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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