5,8,11-Heptadecatrienoic acid, methyl ester

Other names: methyl 5,8,11-heptadecatrienoate
Inchi: InChI=1S/C18H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20-2/h7-8,10-11,
InchiKey: SINQXHSEFNZZNO-SPOHZTNBSA-N
Formula: C18H30O2
SMILES: CCCCCC=CCC=CCC=CCCCC(=O)OC
Mol. weight [g/mol]: 278.43
CAS: 22117-08-4

Physical Properties

Property code	Value	Unit	Source
gf	107.42	kJ/mol	Joback Method
hf	-307.99	kJ/mol	Joback Method
hfus	45.77	kJ/mol	Joback Method
hvap	64.69	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.359		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
ripol	2525.00		NIST Webbook
ripol	2525.00		NIST Webbook
tb	700.01	K	Joback Method
tc	881.96	K	Joback Method
tf	349.54	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.42	J/mol×K	700.01	Joback Method
cpg	740.82	J/mol×K	730.33	Joback Method
cpg	757.37	J/mol×K	760.66	Joback Method
cpg	773.13	J/mol×K	790.98	Joback Method
cpg	788.13	J/mol×K	821.31	Joback Method
cpg	802.42	J/mol×K	851.63	Joback Method

cpg	816.06	J/mol×K	881.96	Joback Method
dvisc	0.0016564	Pa×s	349.54	Joback Method
dvisc	0.0006450	Pa×s	407.95	Joback Method
dvisc	0.0003181	Pa×s	466.36	Joback Method
dvisc	0.0001836	Pa×s	524.77	Joback Method
dvisc	0.0001183	Pa×s	583.19	Joback Method
dvisc	0.0000826	Pa×s	641.60	Joback Method
dvisc	0.0000612	Pa×s	700.01	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=C22117084&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.