

9,12-Hexadecadienoic acid, methyl ester

Inchi:	InChI=1S/C17H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19-2/h5-6,8-9H,3-4,
InchiKey:	VYFSOVMGRZVLMP-HHWLVVFRSA-N
Formula:	C17H30O2
SMILES:	CCCC=CCC=CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	266.42
CAS:	2462-80-8

Physical Properties

Property code	Value	Unit	Source
gf	18.78	kJ/mol	Joback Method
hf	-404.57	kJ/mol	Joback Method
hfus	42.98	kJ/mol	Joback Method
hvap	62.51	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.193		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
tb	672.97	K	Joback Method
tc	850.19	K	Joback Method
tf	343.35	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.37	J/molxK	672.97	Joback Method
cpg	706.83	J/molxK	702.51	Joback Method
cpg	723.48	J/molxK	732.04	Joback Method
cpg	739.33	J/molxK	761.58	Joback Method
cpg	754.44	J/molxK	791.11	Joback Method
cpg	768.82	J/molxK	820.65	Joback Method
cpg	782.53	J/molxK	850.19	Joback Method
dvisc	0.0019334	Paxs	343.35	Joback Method
dvisc	0.0007887	Paxs	398.29	Joback Method

dvisc	0.0003999	Paxs	453.22	Joback Method
dvisc	0.0002348	Paxs	508.16	Joback Method
dvisc	0.0001530	Paxs	563.10	Joback Method
dvisc	0.0001075	Paxs	618.03	Joback Method
dvisc	0.0000801	Paxs	672.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2462808&Units=SI

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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