

16-Methoxy-14-oxohexadec-15-enoic acid, methyl ester

Inchi:	InChI=1S/C18H32O4/c1-21-16-15-17(19)13-11-9-7-5-3-4-6-8-10-12-14-18(20)22-2/h15-1
InchiKey:	NFAZAPLTJBJCEL-FOCLMDBBSA-N
Formula:	C18H32O4
SMILES:	COC=CC(=O)CCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-286.94	kJ/mol	Joback Method
hf	-787.23	kJ/mol	Joback Method
hfus	48.15	kJ/mol	Joback Method
hvap	73.93	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.570		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
tb	767.98	K	Joback Method
tc	950.09	K	Joback Method
tf	431.86	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.20	J/molxK	767.98	Joback Method
cpg	842.07	J/molxK	798.33	Joback Method
cpg	858.05	J/molxK	828.68	Joback Method
cpg	873.15	J/molxK	859.03	Joback Method
cpg	887.40	J/molxK	889.39	Joback Method
cpg	900.81	J/molxK	919.74	Joback Method
cpg	913.41	J/molxK	950.09	Joback Method
dvisc	0.0009629	Paxs	431.86	Joback Method
dvisc	0.0004674	Paxs	487.88	Joback Method
dvisc	0.0002633	Paxs	543.90	Joback Method

dvisc	0.0001651	Paxs	599.92	Joback Method
dvisc	0.0001121	Paxs	655.94	Joback Method
dvisc	0.0000809	Paxs	711.96	Joback Method
dvisc	0.0000613	Paxs	767.98	Joback Method

Sources

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=U191337&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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