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: CO/C=C/C(=O)CCCCCCCCCCCCC(=O)OC

Mol. weight [g/mol]: 312.45

Physical Properties

Property code	Value	Unit	Source
af	0.9469		Cheméo Relay (1.0)
hf	-877.42	kJ/mol	Cheméo Relay (1.0)
hfus	48.15	kJ/mol	Joback Method
hvap	113.94	kJ/mol	Cheméo Relay (1.0)
ie	8.70	eV	Cheméo Relay (1.0)
log10ws	-4.91		Cheméo Relay (1.0)
logp	4.570		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
tb	600.96	K	Cheméo Relay (1.0)
tc	786.85	K	Cheméo Relay (1.0)
tf	339.77	K	Cheméo Relay (1.0)
vc	1.034	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0002633	Pa×s	543.90	Joback Method
dvisc	0.0001651	Pa×s	599.92	Joback Method
dvisc	0.0001121	Pa×s	655.94	Joback Method
dvisc	0.0000809	Pa×s	711.96	Joback Method
dvisc	0.0000613	Pa×s	767.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U191337&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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