7,10,13-Hexadecatrienoic acid, methyl ester

Other names: Methyl 7,10,13-hexadecatrienoate
Inchi: InChI=1S/C17H28O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19-2/h4-5,7-8,10-11
InchiKey: DUOCBVNCDAEWTB-JSIPCRQOSA-N
Formula: C17H28O2
SMILES: CCC=CCC=CCC=CCCCCCC(=O)OC
Mol. weight [g/mol]: 264.40
CAS: 56554-30-4

Physical Properties

Property code	Value	Unit	Source
gf	99.00	kJ/mol	Joback Method
hf	-287.35	kJ/mol	Joback Method
hfus	43.18	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.969		Crippen Method
mcvol	244.930	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
ripol	2380.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2380.00		NIST Webbook
tb	677.13	K	Joback Method
tc	859.74	K	Joback Method
tf	338.27	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.53	J/mol×K	677.13	Joback Method
cpg	684.55	J/mol×K	707.56	Joback Method
cpg	700.73	J/mol×K	738.00	Joback Method
cpg	716.12	J/mol×K	768.43	Joback Method
cpg	730.77	J/mol×K	798.87	Joback Method

cpg	744.71	J/mol×K	829.30	Joback Method
cpg	758.01	J/mol×K	859.74	Joback Method
dvisc	0.0018095	Pa×s	338.27	Joback Method
dvisc	0.0007111	Pa×s	394.75	Joback Method
dvisc	0.0003531	Pa×s	451.22	Joback Method
dvisc	0.0002049	Pa×s	507.70	Joback Method
dvisc	0.0001325	Pa×s	564.18	Joback Method
dvisc	0.0000928	Pa×s	620.65	Joback Method
dvisc	0.0000690	Pa×s	677.13	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C56554304&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume