3,6-Dodecadienoic acid, methyl ester

Other names: Methyl 3,6-dodecadienoate
Inchi: InChI=1S/C13H22O2/c1-3-4-5-6-7-8-9-10-11-12-13(14)15-2/h7-8,10-11H,3-6,9,12H2,1-2
InchiKey: QOLQXDRXMBPSFD-ZDVGBALWSA-N
Formula: C13H22O2
SMILES: CCCCCC=CCC=CCC(=O)OC
Mol. weight [g/mol]: 210.31
CAS: 16106-01-7

Physical Properties

Property code	Value	Unit	Source
gf	-14.90	kJ/mol	Joback Method
hf	-322.01	kJ/mol	Joback Method
hfus	32.62	kJ/mol	Joback Method
hvap	53.60	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.632		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1482.00		NIST Webbook
tb	581.45	K	Joback Method
tc	763.24	K	Joback Method
tf	298.27	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.55	J/mol×K	581.45	Joback Method
cpg	492.11	J/mol×K	611.75	Joback Method
cpg	506.92	J/mol×K	642.05	Joback Method
cpg	521.03	J/mol×K	672.35	Joback Method
cpg	534.46	J/mol×K	702.64	Joback Method
cpg	547.24	J/mol×K	732.94	Joback Method
cpg	559.41	J/mol×K	763.24	Joback Method

dvisc	0.0025562	Pa×s	298.27	Joback Method
dvisc	0.0010928	Pa×s	345.47	Joback Method
dvisc	0.0005731	Pa×s	392.66	Joback Method
dvisc	0.0003452	Pa×s	439.86	Joback Method
dvisc	0.0002294	Pa×s	487.06	Joback Method
dvisc	0.0001638	Pa×s	534.25	Joback Method
dvisc	0.0001236	Pa×s	581.45	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=C16106017&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume