(Z,E)-9,11-Tetradecadienyl acetate

Inchi: InChI=1S/C16H28O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-16(2)17/h4-7H,3,8-15H2,1-
InchiKey: RFEQLTBBKNKGGJ-RZSVFLSASA-N
Formula: C16H28O2
SMILES: CCC=CC=CCCCCCCCCOC(C)=O
Mol. weight [g/mol]: 252.39

Physical Properties

Property code	Value	Unit	Source
gf	10.36	kJ/mol	Joback Method
hf	-383.93	kJ/mol	Joback Method
hfus	40.39	kJ/mol	Joback Method
hvap	60.28	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.803		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1834.00		NIST Webbook
rinpol	1834.00		NIST Webbook
ripol	2202.00		NIST Webbook
tb	650.09	K	Joback Method
tc	827.94	K	Joback Method
tf	332.08	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.12	J/mol×K	650.09	Joback Method
cpg	651.17	J/mol×K	679.73	Joback Method
cpg	667.42	J/mol×K	709.37	Joback Method
cpg	682.90	J/mol×K	739.01	Joback Method
cpg	697.64	J/mol×K	768.65	Joback Method
cpg	711.69	J/mol×K	798.30	Joback Method
cpg	725.06	J/mol×K	827.94	Joback Method

dvisc	0.0020986	Pa×s	332.08	Joback Method
dvisc	0.0008652	Pa×s	385.08	Joback Method
dvisc	0.0004420	Pa×s	438.08	Joback Method
dvisc	0.0002610	Pa×s	491.09	Joback Method
dvisc	0.0001708	Pa×s	544.09	Joback Method
dvisc	0.0001205	Pa×s	597.09	Joback Method
dvisc	0.0000900	Pa×s	650.09	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=R490805&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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