

9,11-Tetradecadien-1-ol, acetate

Other names:	(9E,11E)-tetradeca-9,11-dienyl 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-YTXXJHMSA-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	1810.00		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	725.06	J/molxK	827.94	Joback Method
cpg	634.12	J/molxK	650.09	Joback Method
cpg	651.17	J/molxK	679.73	Joback Method
cpg	667.42	J/molxK	709.37	Joback Method
cpg	682.90	J/molxK	739.01	Joback Method
cpg	697.64	J/molxK	768.65	Joback Method
cpg	711.69	J/molxK	798.30	Joback Method
dvisc	0.0000900	Paxs	650.09	Joback Method

dvisc	0.0020986	Paxs	332.08	Joback Method
dvisc	0.0008652	Paxs	385.08	Joback Method
dvisc	0.0004420	Paxs	438.08	Joback Method
dvisc	0.0002610	Paxs	491.09	Joback Method
dvisc	0.0001708	Paxs	544.09	Joback Method
dvisc	0.0001205	Paxs	597.09	Joback Method
hvapt	92.30	kJ/mol	298.15	The Vaporization Enthalpies and Vapor Pressures of Some Insect Pheromones by Correlation Gas Chromatography

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R308602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Vaporization Enthalpies and Vapor Pressures of Some Insect Pheromones by Correlation Gas Chromatography:	https://www.doi.org/10.1021/acs.jced.5b00892
	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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

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