

10,12-Hexadecadien-1-ol, acetate

Inchi:	InChI=1S/C18H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-18(2)19/h5-8H,3-4,9
InchiKey:	CMCBHGAXGCXMIP-BSWSSELBSA-N
Formula:	C18H32O2
SMILES:	CCCC=CC=CCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	280.45

Physical Properties

Property code	Value	Unit	Source
gf	27.20	kJ/mol	Joback Method
hf	-425.21	kJ/mol	Joback Method
hfus	45.57	kJ/mol	Joback Method
hvap	64.73	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.583		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	695.85	K	Joback Method
tc	872.86	K	Joback Method
tf	354.62	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.84	J/molxK	695.85	Joback Method
cpg	763.70	J/molxK	725.35	Joback Method
cpg	780.72	J/molxK	754.85	Joback Method
cpg	796.93	J/molxK	784.36	Joback Method
cpg	812.37	J/molxK	813.86	Joback Method
cpg	827.07	J/molxK	843.36	Joback Method
cpg	841.08	J/molxK	872.86	Joback Method
dvisc	0.0017692	Paxs	354.62	Joback Method

dvisc	0.0007146	Paxs	411.49	Joback Method
dvisc	0.0003597	Paxs	468.36	Joback Method
dvisc	0.0002101	Paxs	525.24	Joback Method
dvisc	0.0001363	Paxs	582.11	Joback Method
dvisc	0.0000955	Paxs	638.98	Joback Method
dvisc	0.0000709	Paxs	695.85	Joback Method

Sources

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=R308528&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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