11,13-Dimethyl-12-tetradecen-1-ol acetate

Inchi: InChI=1S/C18H34O2/c1-16(2)15-17(3)13-11-9-7-5-6-8-10-12-14-20-18(4)19/h15,17H,5-1
InchiKey: MNUWBCKALSZWEW-UHFFFAOYSA-N
Formula: C18H34O2
SMILES: CC(=O)OCCCCCCCCCCCC(C)C=C(C)C
Mol. weight [g/mol]: 282.46

Physical Properties

Property code	Value	Unit	Source
gf	-64.01	kJ/mol	Joback Method
hf	-557.50	kJ/mol	Joback Method
hfus	40.53	kJ/mol	Joback Method
hvap	64.47	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.663		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	1955.10		NIST Webbook
rinpol	1955.10		NIST Webbook
tb	691.13	K	Joback Method
tc	867.34	K	Joback Method
tf	330.74	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.10	J/mol×K	691.13	Joback Method
cpg	786.83	J/mol×K	720.50	Joback Method
cpg	804.68	J/mol×K	749.87	Joback Method
cpg	821.68	J/mol×K	779.23	Joback Method
cpg	837.85	J/mol×K	808.60	Joback Method
cpg	853.24	J/mol×K	837.97	Joback Method
cpg	867.86	J/mol×K	867.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U130810&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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