1,5-dimethyl-1-vinylhept-4-enyl acetate

Other names: 1,6-Nonadien-3-ol, 3,7-dimethyl-, acetate
Inchi: InChI=1S/C13H22O2/c1-6-11(3)9-8-10-13(5,7-2)15-12(4)14/h7,9H,2,6,8,10H2,1,3-5H3/b
InchiKey: IVSZEHYDOLAREK-PKNBQFBNSA-N
Formula: C13H22O2
SMILES: C=CC(C)(CCC=C(C)CC)OC(C)=O
Mol. weight [g/mol]: 210.31
CAS: 61931-80-4

Physical Properties

Property code	Value	Unit	Source
gf	-12.99	kJ/mol	Joback Method
hf	-332.34	kJ/mol	Joback Method
hfus	22.41	kJ/mol	Joback Method
hvap	51.76	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.631		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	1346.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1344.00		NIST Webbook
tb	570.62	K	Joback Method
tc	761.16	K	Joback Method
tf	290.05	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.02	J/mol×K	570.62	Joback Method
cpg	494.53	J/mol×K	602.38	Joback Method
cpg	510.14	J/mol×K	634.13	Joback Method
cpg	524.91	J/mol×K	665.89	Joback Method
cpg	538.88	J/mol×K	697.65	Joback Method

cpg	552.08	J/mol×K	729.40	Joback Method
cpg	564.56	J/mol×K	761.16	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=C61931804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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