4,7-Methano-1H-inden-6-ol, 3a,4,5,6,7,7a-hexahydro-, acetate

Other names: Verdyl acetate
4,7-Methanoinden-6-ol, 3a,4,5,6,7,7a-hexahydro-, acetate
Dihydro-nordicyclopentadienyl acetate
Tricyclodecen-4-yl 8-acetate
3a,4,5,6,7,7a-hexahydro-4,7-methanoinden-6-yl acetate

Inchi: InChI=1S/C12H16O2/c1-7(13)14-12-6-8-5-11(12)10-4-2-3-9(8)10/h2-3,8-12H,4-6H2,1H3

InchiKey: RGVQNSFGUOIKFF-UHFFFAOYSA-N

Formula: C12H16O2

SMILES: CC(=O)OC1CC2CC1C1CC=CC21

Mol. weight [g/mol]: 192.25

CAS: 5413-60-5

Physical Properties

Property code	Value	Unit	Source
gf	0.93	kJ/mol	Joback Method
hf	-306.47	kJ/mol	Joback Method
hfus	25.29	kJ/mol	Joback Method
hvap	51.05	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.150		Crippen Method
mcvol	150.500	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1406.00		NIST Webbook
rinpol	1406.70		NIST Webbook
rinpol	1407.00		NIST Webbook
ripol	1881.00		NIST Webbook
tb	564.56	K	Joback Method
tc	780.81	K	Joback Method
tf	339.74	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	407.03	J/mol×K	564.56	Joback Method
cpg	425.84	J/mol×K	600.60	Joback Method
cpg	443.41	J/mol×K	636.64	Joback Method
cpg	459.82	J/mol×K	672.68	Joback Method
cpg	475.14	J/mol×K	708.72	Joback Method
cpg	489.45	J/mol×K	744.76	Joback Method
cpg	502.84	J/mol×K	780.81	Joback Method
dvisc	0.0018650	Pa×s	339.74	Joback Method
dvisc	0.0019297	Pa×s	377.21	Joback Method
dvisc	0.0019844	Pa×s	414.68	Joback Method
dvisc	0.0020312	Pa×s	452.15	Joback Method
dvisc	0.0020717	Pa×s	489.62	Joback Method
dvisc	0.0021070	Pa×s	527.09	Joback Method
dvisc	0.0021382	Pa×s	564.56	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5413605&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

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