

Nerolidyl acetate

Other names:	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, acetate Nerolidol, acetate 3,7,11-Trimethyl-1,6,10-dodecatrien-3-yl acetate 3,7,11-trimethyldodeca-1,6,10-trien-3-yl acetate
Inchi:	InChI=1S/C17H28O2/c1-7-17(6,19-16(5)18)13-9-12-15(4)11-8-10-14(2)3/h7,10,12H,1,8-
InchiKey:	PRNJXUQTUSFYLV-UHFFFAOYSA-N
Formula:	C17H28O2
SMILES:	C=CC(C)(CCC=C(C)CCC=C(C)C)OC(C)=O
Mol. weight [g/mol]:	264.40
CAS:	2306-78-7

Physical Properties

Property code	Value	Unit	Source
gf	92.36	kJ/mol	Joback Method
hf	-307.47	kJ/mol	Joback Method
hfus	31.66	kJ/mol	Joback Method
hvap	60.70	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.967		Crippen Method
mcvol	244.930	ml/mol	McGowan Method
pc	1446.83	kPa	Joback Method
rinpol	1687.00		NIST Webbook
rinpol	1687.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2271.00		NIST Webbook
tb	666.18	K	Joback Method
tc	858.25	K	Joback Method
tf	316.09	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	667.79	J/mol×K	666.18	Joback Method
cpg	685.72	J/mol×K	698.19	Joback Method
cpg	702.68	J/mol×K	730.20	Joback Method
cpg	718.71	J/mol×K	762.22	Joback Method
cpg	733.89	J/mol×K	794.23	Joback Method
cpg	748.27	J/mol×K	826.24	Joback Method
cpg	761.92	J/mol×K	858.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2306787&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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