

(Z)-Nerolidyl acetate

Other names:	(Z)-«beta»-Nerolidyl acetate cis-Nerolidyl 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-QINSGFPZSA-N
Formula:	C17H28O2
SMILES:	<chem>C=CC(C)(CCC=C(C)CCC=C(C)C)OC(C)=O</chem>
Mol. weight [g/mol]:	264.40
CAS:	91050-14-5

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	1675.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1655.00		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
cpg	667.79	J/molxK	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/ci9903071
Crippen Method:	https://www.cheméo.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=C91050145&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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