

Nerolidyl propionate

Other names:trans-nerolidyl propanoate

Inchi:InChI=1S/C18H30O2/c1-7-17(19)20-18(6,8-2)14-10-13-16(5)12-9-11-15(3)4/h8,11,13H,2

InchiKey:NPSBIIPKEQTFPA-SSZFMOIBSA-N

Formula:C18H30O2

SMILES:C=CC(C)(CCC=C(C)CCC=C(C)C)OC(=O)CC

Mol. weight [g/mol]:278.43

Physical Properties

Property code	Value	Unit	Source
gf	100.78	kJ/mol	Joback Method
hf	-328.11	kJ/mol	Joback Method
hfus	34.25	kJ/mol	Joback Method
hvap	62.93	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.357		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
pc	1346.69	kPa	Joback Method
rinpol	1829.00		NIST Webbook
rinpol	1829.00		NIST Webbook
rinpol	1850.00		NIST Webbook
tb	689.06	K	Joback Method
tc	879.50	K	Joback Method
tf	327.36	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.33	J/mol×K	689.06	Joback Method
cpg	741.55	J/mol×K	720.80	Joback Method
cpg	758.80	J/mol×K	752.54	Joback Method
cpg	775.14	J/mol×K	784.28	Joback Method
cpg	790.61	J/mol×K	816.02	Joback Method
cpg	805.30	J/mol×K	847.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U132164&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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