

Nopyl acetate

Other names:	Bicyclo[3.1.1]hept-2-ene-2-ethanol, 6,6-dimethyl-, acetate Citroviol Lignyl acetate Nopol acetate 2-Norpinene-2-ethanol, 6,6-dimethyl-, acetate 2-Pinene-10-methyl acetate 6,6-Dimethyl-2-norpinene-2-ethanol, acetate 6,6-Dimethylbicyclo(3.1.1)-2-heptene-2-ethyl acetate
Inchi:	InChI=1S/C13H20O2/c1-9(14)15-7-6-10-4-5-11-8-12(10)13(11,2)3/h4,11-12H,5-8H2,1-3H
InchiKey:	AWNOGHRWORTNEI-UHFFFAOYSA-N
Formula:	C13H20O2
SMILES:	CC(=O)OCCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]:	208.30
CAS:	128-51-8

Physical Properties

Property code	Value	Unit	Source
gf	-58.81	kJ/mol	Joback Method
hf	-375.80	kJ/mol	Joback Method
hfus	21.99	kJ/mol	Joback Method
hvap	53.18	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.932		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1413.10		NIST Webbook
rinpol	1412.00		NIST Webbook
ripol	1777.00		NIST Webbook
ripol	1777.00		NIST Webbook
tb	590.59	K	Joback Method
tc	797.71	K	Joback Method
tf	373.73	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.54	J/mol×K	590.59	Joback Method
cpg	486.01	J/mol×K	625.11	Joback Method
cpg	502.50	J/mol×K	659.63	Joback Method
cpg	518.12	J/mol×K	694.15	Joback Method
cpg	533.01	J/mol×K	728.67	Joback Method
cpg	547.29	J/mol×K	763.19	Joback Method
cpg	561.07	J/mol×K	797.71	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=C128518&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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