

cis-Verbenyl acetate

Other names:	(Z)-Verbenyl acetate
Inchi:	InChI=1S/C12H18O2/c1-7-5-11(14-8(2)13)10-6-9(7)12(10,3)4/h5,9-11H,6H2,1-4H3/t9?,1
InchiKey:	OZBFUQLOVFXDNK-VQXHTEKXSA-N
Formula:	C12H18O2
SMILES:	CC(=O)OC1C=C(C)C2CC1C2(C)C
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
gf	-74.94	kJ/mol	Joback Method
hf	-375.50	kJ/mol	Joback Method
hfus	20.47	kJ/mol	Joback Method
hvap	50.64	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1278.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1280.00		NIST Webbook
tb	563.04	K	Joback Method
tc	773.40	K	Joback Method
tf	358.22	K	Joback Method
vc	0.620	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.92	J/molxK	563.04	Joback Method
cpg	437.32	J/molxK	598.10	Joback Method
cpg	453.71	J/molxK	633.16	Joback Method
cpg	469.20	J/molxK	668.22	Joback Method
cpg	483.90	J/molxK	703.28	Joback Method
cpg	497.94	J/molxK	738.34	Joback Method
cpg	511.43	J/molxK	773.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R129929&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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