

Citronellyl vinyl ether

Inchi:	InChI=1S/C12H22O/c1-5-13-10-9-12(4)8-6-7-11(2)3/h5,7,12H,1,6,8-10H2,2-4H3
InchiKey:	PWCLCTUZQHYTKS-UHFFFAOYSA-N
Formula:	C12H22O
SMILES:	<chem>C=COCCC(C)CCC=C(C)C</chem>
Mol. weight [g/mol]:	182.30

Physical Properties

Property code	Value	Unit	Source
gf	102.23	kJ/mol	Joback Method
hf	-195.65	kJ/mol	Joback Method
hfus	22.11	kJ/mol	Joback Method
hvap	43.70	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.919		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	1235.00		NIST Webbook
rinpol	1235.00		NIST Webbook
ripol	1445.00		NIST Webbook
tb	496.66	K	Joback Method
tc	673.95	K	Joback Method
tf	211.43	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.59	J/molxK	496.66	Joback Method
cpg	416.96	J/molxK	526.21	Joback Method
cpg	432.62	J/molxK	555.76	Joback Method
cpg	447.60	J/molxK	585.30	Joback Method
cpg	461.92	J/molxK	614.85	Joback Method
cpg	475.59	J/molxK	644.40	Joback Method
cpg	488.65	J/molxK	673.95	Joback Method

Sources

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=R409582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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