

Geranyl ethyl ether 1

Other names:	Nerylethyl ether
Inchi:	InChI=1S/C12H22O/c1-5-13-10-9-12(4)8-6-7-11(2)3/h7,9H,5-6,8,10H2,1-4H3/b12-9+
InchiKey:	LOUIMJFJROISMD-FMIVXFBMSA-N
Formula:	C12H22O
SMILES:	CCOCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	182.30

Physical Properties

Property code	Value	Unit	Source
gf	88.50	kJ/mol	Joback Method
hf	-208.37	kJ/mol	Joback Method
hfus	25.81	kJ/mol	Joback Method
hvap	44.79	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.716		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
tb	504.46	K	Joback Method
tc	685.53	K	Joback Method
tf	209.15	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.82	J/molxK	504.46	Joback Method
cpg	418.27	J/molxK	534.64	Joback Method
cpg	433.98	J/molxK	564.82	Joback Method
cpg	448.97	J/molxK	595.00	Joback Method
cpg	463.28	J/molxK	625.17	Joback Method
cpg	476.92	J/molxK	655.35	Joback Method
cpg	489.94	J/molxK	685.53	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=U285275&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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