Geranyl 2-butyl ether

Inchi: InChI=1S/C14H26O/c1-6-14(5)15-11-10-13(4)9-7-8-12(2)3/h8,10,14H,6-7,9,11H2,1-5H3/
InchiKey: YGQWCPGGYPONFL-JLHYYAGUSA-N
Formula: C14H26O
SMILES: CCC(C)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 210.36

Physical Properties

Property code	Value	Unit	Source
gf	102.90	kJ/mol	Joback Method
hf	-254.93	kJ/mol	Joback Method
hfus	27.47	kJ/mol	Joback Method
hvap	48.86	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.494		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	1466.00		NIST Webbook
tb	549.78	K	Joback Method
tc	730.81	K	Joback Method
tf	216.69	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.48	J/mol×K	549.78	Joback Method
cpg	518.59	J/mol×K	579.95	Joback Method
cpg	535.86	J/mol×K	610.12	Joback Method
cpg	552.34	J/mol×K	640.29	Joback Method
cpg	568.05	J/mol×K	670.47	Joback Method
cpg	583.03	J/mol×K	700.64	Joback Method
cpg	597.31	J/mol×K	730.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R570253&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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