

Hydroxygermacrene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H26O/c1-12-5-4-6-13(2)8-10-15(9-7-12)14(3)11-16/h5,8,14-16H,4,6-7,9-11

RGQPCXBXPJFJIT-TWHNSCTMSA-N

C15H26O

CC1=CCC(C(C)CO)CCC(C)=CCC1

222.37

Physical Properties

Property code	Value	Unit	Source
gf	-47.13	kJ/mol	Joback Method
hf	-388.14	kJ/mol	Joback Method
hfus	20.27	kJ/mol	Joback Method
hvap	68.30	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.088		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1564.00		NIST Webbook
tb	679.25	K	Joback Method
tc	885.81	K	Joback Method
tf	324.49	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.28	J/mol×K	679.25	Joback Method
cpg	617.10	J/mol×K	713.68	Joback Method
cpg	635.72	J/mol×K	748.10	Joback Method
cpg	653.14	J/mol×K	782.53	Joback Method
cpg	669.37	J/mol×K	816.96	Joback Method
cpg	684.42	J/mol×K	851.39	Joback Method
cpg	698.28	J/mol×K	885.81	Joback Method
dvisc	0.0109949	Pa×s	324.49	Joback Method
dvisc	0.0015213	Pa×s	383.62	Joback Method

dvisc	0.0003570	Pa×s	442.74	Joback Method
dvisc	0.0001179	Pa×s	501.87	Joback Method
dvisc	0.0000492	Pa×s	561.00	Joback Method
dvisc	0.0000242	Pa×s	620.12	Joback Method
dvisc	0.0000135	Pa×s	679.25	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=R200167&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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