

Germacrene A

Inchi:

InChI=1S/C14H22/c1-12(2)14-9-7-5-4-6-8-13(3)10-11-14/h5,7-8,14H,1,4,6,9-11H2,2-3H3

InchiKey:

XNNFTAIJLZPUAI-HNVHAEGFSA-N

Formula:

C14H22

SMILES:

C=C(C)C1CC=CCCC=C(C)CC1

Mol. weight [g/mol]:

190.32

CAS:

28387-44-2

Physical Properties

Property code	Value	Unit	Source
gf	172.63	kJ/mol	Joback Method
hf	-82.88	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	48.53	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.645		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	1476.00		NIST Webbook
rinpol	1509.00		NIST Webbook
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rinpol	1503.00		NIST Webbook
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ripol	1741.00		NIST Webbook
ripol	1757.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1747.00		NIST Webbook
tb	556.21	K	Joback Method
tc	785.86	K	Joback Method
tf	239.16	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.33	J/mol×K	556.21	Joback Method
cpg	470.16	J/mol×K	594.48	Joback Method
cpg	492.58	J/mol×K	632.76	Joback Method
cpg	513.60	J/mol×K	671.03	Joback Method
cpg	533.26	J/mol×K	709.31	Joback Method
cpg	551.56	J/mol×K	747.58	Joback Method
cpg	568.51	J/mol×K	785.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28387442&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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