

(-)-Germacrene D

Inchi:	InChI=1S/C15H24/c1-12(2)15-10-8-13(3)6-5-7-14(4)9-11-15/h7-8,10,12,15H,3,5-6,9,11H
InchiKey:	GAIBLDCXCZKKJE-LVVNOCGRSA-N
Formula:	C15H24
SMILES:	<chem>C=C1C=CC(C(C)C)CCC(C)=CCC1</chem>
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	152.40	kJ/mol	Joback Method
hf	-140.20	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.891		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1482.00		NIST Webbook
tb	581.25	K	Joback Method
tc	804.50	K	Joback Method
tf	264.83	K	Joback Method
vc	0.727	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.53	J/molxK	581.25	Joback Method
cpg	604.19	J/molxK	767.29	Joback Method
cpg	585.93	J/molxK	730.09	Joback Method
cpg	566.34	J/molxK	692.88	Joback Method
cpg	545.41	J/molxK	655.67	Joback Method
cpg	523.14	J/molxK	618.46	Joback Method
cpg	621.12	J/molxK	804.50	Joback Method
dvisc	0.0000689	Paxs	581.25	Joback Method

dvisc	0.0001030	Paxs	528.51	Joback Method
dvisc	0.0001684	Paxs	475.78	Joback Method
dvisc	0.0003112	Paxs	423.04	Joback Method
dvisc	0.0006848	Paxs	370.30	Joback Method
dvisc	0.0019587	Paxs	317.57	Joback Method
dvisc	0.0085131	Paxs	264.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R405446&Units=SI

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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