

(+)-Germacrene A

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24/c1-12(2)15-10-8-13(3)6-5-7-14(4)9-11-15/h6,9,15H,1,5,7-8,10-11H2,2

XMRKUJJDDKYUHV-SDFJSLCBSA-N

C15H24

C=C(C)C1CC=C(C)CCC=C(C)CC1

204.35

Physical Properties

Property code	Value	Unit	Source
gf	171.42	kJ/mol	Joback Method
hf	-114.99	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1501.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1506.00		NIST Webbook
tb	584.07	K	Joback Method
tc	810.41	K	Joback Method
tf	262.95	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.67	J/mol×K	584.07	Joback Method
cpg	523.53	J/mol×K	621.79	Joback Method
cpg	546.01	J/mol×K	659.52	Joback Method
cpg	567.11	J/mol×K	697.24	Joback Method

cpg	586.84	J/mol×K	734.97	Joback Method
cpg	605.21	J/mol×K	772.69	Joback Method
cpg	622.25	J/mol×K	810.41	Joback Method

Sources

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=R336711&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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