

Germacrene C

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/h6,9,11-12H,5,7-8,10H2,1-4

WYGLLWYGQRUNLF-VUSWODRPSA-N

C15H24

CC1=CC=C(C(C)C)CCC(C)=CCC1

204.35

Physical Properties

Property code	Value	Unit	Source
gf	117.73	kJ/mol	Joback Method
hf	-169.26	kJ/mol	Joback Method
hfus	15.95	kJ/mol	Joback Method
hvap	52.88	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	1516.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1493.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1754.00		NIST Webbook
ripol	1754.00		NIST Webbook
ripol	1754.00		NIST Webbook
tb	595.88	K	Joback Method
tc	821.36	K	Joback Method
tf	281.19	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.78	J/mol×K	595.88	Joback Method
cpg	523.38	J/mol×K	633.46	Joback Method
cpg	544.66	J/mol×K	671.04	Joback Method
cpg	564.65	J/mol×K	708.62	Joback Method
cpg	583.34	J/mol×K	746.20	Joback Method
cpg	600.74	J/mol×K	783.78	Joback Method
cpg	616.87	J/mol×K	821.36	Joback Method
dvisc	0.0062064	Pa×s	281.19	Joback Method
dvisc	0.0014960	Pa×s	333.64	Joback Method
dvisc	0.0005307	Pa×s	386.09	Joback Method
dvisc	0.0002413	Pa×s	438.53	Joback Method
dvisc	0.0001298	Pa×s	490.98	Joback Method
dvisc	0.0000787	Pa×s	543.43	Joback Method
dvisc	0.0000521	Pa×s	595.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R203384&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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