

1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-

Other names: 7,11-Dimethyl-3-methylene-1,6,10-dodecatriene

«beta»-Farnesene

7,11-dimethyl-3-methylenedodeca-1,6,10-triene

Inchi:

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

InchiKey:

JSNRRGGBADWTMC-NTCAYCPXSA-N

Formula:

C15H24

SMILES:

C=CC(=C)CCC=C(C)CCC=C(C)C

Mol. weight [g/mol]:

204.35

CAS:

77129-48-7

Physical Properties

Property code	Value	Unit	Source
gf	385.89	kJ/mol	Joback Method
hf	103.00	kJ/mol	Joback Method
hfus	28.52	kJ/mol	Joback Method
hvap	47.80	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.202		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1446.00		NIST Webbook
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tb	543.92	K	Joback Method
tc	730.22	K	Joback Method
tf	203.25	K	Joback Method
vc	0.800	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.95	J/molxK	543.92	Joback Method
cpg	499.95	J/molxK	574.97	Joback Method
cpg	517.00	J/molxK	606.02	Joback Method
cpg	533.16	J/molxK	637.07	Joback Method
cpg	548.48	J/molxK	668.12	Joback Method
cpg	563.01	J/molxK	699.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77129487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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