cis-«beta»-Farnesene

Other names:	1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-, (Z)- (Z)-«beta»-Farnesene (6Z)-7,11-Dimethyl-3-methylene-1,6,10-dodecatriene «beta»-cis-Farnesene «beta»-(Z)-Farnesene
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-QINSGFPZSA-N
Formula:	C15H24
SMILES:	C=CC(=C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	204.35
CAS:	28973-97-9

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	1433.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1443.00		NIST Webbook
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ripol	1633.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1630.00		NIST Webbook
tb	543.92	K	Joback Method
tc	730.22	K	Joback Method
tf	203.25	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.95	J/mol×K	543.92	Joback Method
cpg	499.95	J/mol×K	574.97	Joback Method
cpg	517.00	J/mol×K	606.02	Joback Method
cpg	533.16	J/mol×K	637.07	Joback Method
cpg	548.48	J/mol×K	668.12	Joback Method
cpg	563.01	J/mol×K	699.17	Joback Method
cpg	576.82	J/mol×K	730.22	Joback Method

Sources

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=C28973979&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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