

«beta»-Bisabolene

Other names:

Cyclohexene, 1-methyl-4-(5-methyl-1-methylene-4-hexenyl)-, (S)-
1,5-Heptadiene, 6-methyl-2-(4-methyl-3-cyclohexen-1-yl)-, (S)-(-)-
l-«beta»-Bisabolene
(+,-)-«beta»-Bisabolene
1-Methyl-4-(5-methyl-1-methylene-4-hexenyl)-1-cyclohexene-, (4S)-
beta-Bisabolene
(-)-«beta»-bisabolene
1-Methyl-4-(5-methyl-1-methylene-4-hexenyl)-(S)-cyclohexene
Cyclohexene, 1-methyl-4-(5-methyl-1-methylene-4-hexen-1-yl)-, (4S)-

Inchi: InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6,8,15H,4-5,7,9-11H2,1-3H3**InchiKey:** XZRVRYFILCSYSP-HNNXBMFYSA-N**Formula:** C15H24**SMILES:** C=C(CCC=C(C)C)C1CC=C(C)CC1**Mol. weight [g/mol]:** 204.35**CAS:** 495-61-4

Physical Properties

Property code	Value	Unit	Source
gf	271.16	kJ/mol	Joback Method
hf	-29.23	kJ/mol	Joback Method
hfus	23.58	kJ/mol	Joback Method
hvap	49.81	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
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ripol	1746.00		NIST Webbook
ripol	1736.00		NIST Webbook
tb	566.89	K	Joback Method
tc	773.75	K	Joback Method
tf	244.71	K	Joback Method
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.97	J/mol×K	566.89	Joback Method
cpg	513.94	J/mol×K	601.37	Joback Method
cpg	533.73	J/mol×K	635.84	Joback Method
cpg	552.38	J/mol×K	670.32	Joback Method
cpg	569.95	J/mol×K	704.80	Joback Method
cpg	586.51	J/mol×K	739.28	Joback Method
cpg	602.09	J/mol×K	773.75	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=C495614&Units=SI

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
mccvol:	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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