

Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-

Other names: «beta»-Sesquiphellandrene
3-((1S)-1,5-Dimethyl-4-hexenyl)-6-methylene-1-cyclohexene, (3R)-
(-)-«beta»-Sesquiphellandrene
«beta»-Sesquiphellanderene

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

InchiKey: PHWISBHSBNDZDX-YSSOQSIOSA-N

Formula: C15H24

SMILES: C=C1C=CC(C(C)CCC=C(C)C)CC1

Mol. weight [g/mol]: 204.35

CAS: 20307-83-9

Physical Properties

Property code	Value	Unit	Source
gf	252.14	kJ/mol	Joback Method
hf	-54.44	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	49.51	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.891		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
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ripol	1783.00		NIST Webbook
tb	564.07	K	Joback Method
tc	768.15	K	Joback Method
tf	246.59	K	Joback Method

vc	0.753	m3/kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.92	J/mol×K	564.07	Joback Method
cpg	513.68	J/mol×K	598.08	Joback Method
cpg	533.28	J/mol×K	632.10	Joback Method
cpg	551.78	J/mol×K	666.11	Joback Method
cpg	569.23	J/mol×K	700.12	Joback Method
cpg	585.67	J/mol×K	734.14	Joback Method
cpg	601.14	J/mol×K	768.15	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=C20307839&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
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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