cis-«alpha»-Bisabolene

Other names: 4-[(1Z)-1,5-Dimethyl-1,4-hexadienyl]-1-methyl-1-cyclohexene
«alpha»-Bisabolene (Z)
(Z)-«alpha»-Bisabolene
Cyclohexene, 4-[(1Z)-1,5-dimethyl-1,4-hexadien-1-yl]-1-methyl-
2,5-Heptadiene, 2-methyl-6-(4-methyl-3-cyclohexen-1-yl)-, (Z)-
Cyclohexene, 4-(1,5-dimethyl-1,4-hexadienyl)-1-methyl-, (Z)-
(Z)-«alpha»-Bisabilene

Inchi: InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6-8,15H,5,9-11H2,1-4H3/b

InchiKey: YHBUQBJHSRGZNF-AUWJEWJLSA-N

Formula: C15H24

SMILES: CC(C)=CCC=C(C)C1CC=C(C)CC1

Mol. weight [g/mol]: 204.35

CAS: 29837-07-8

Physical Properties

Property code	Value	Unit	Source
gf	263.54	kJ/mol	Joback Method
hf	-37.44	kJ/mol	Joback Method
hfus	25.06	kJ/mol	Joback Method
hvap	50.44	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1508.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1495.00		NIST Webbook

rinpol	1511.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1501.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1521.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1494.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1495.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1509.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1495.00	NIST Webbook
rinpol	1496.00	NIST Webbook
rinpol	1496.00	NIST Webbook
rinpol	1509.00	NIST Webbook
rinpol	1495.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1499.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1498.00	NIST Webbook
rinpol	1501.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1493.00	NIST Webbook
rinpol	1479.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1509.00	NIST Webbook
rinpol	1492.00	NIST Webbook
rinpol	1499.00	NIST Webbook
rinpol	1498.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1503.00	NIST Webbook
ripol	1759.00	NIST Webbook
ripol	1727.00	NIST Webbook
ripol	1702.00	NIST Webbook
ripol	1724.00	NIST Webbook
ripol	1719.00	NIST Webbook
ripol	1761.00	NIST Webbook
ripol	1740.00	NIST Webbook
ripol	1759.00	NIST Webbook

ripol	1719.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	1772.00		NIST Webbook
ripol	1761.00		NIST Webbook
tb	574.37	K	Joback Method
tc	785.97	K	Joback Method
tf	241.39	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.01	J/mol×K	574.37	Joback Method
cpg	516.16	J/mol×K	609.64	Joback Method
cpg	536.07	J/mol×K	644.90	Joback Method
cpg	554.80	J/mol×K	680.17	Joback Method
cpg	572.42	J/mol×K	715.43	Joback Method
cpg	589.00	J/mol×K	750.70	Joback Method
cpg	604.60	J/mol×K	785.97	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29837078&Units=SI
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

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