

(R)-1-Methyl-4-(6-methylhept-5-en-2-yl)cyclohexa-

Other names:	«beta»-Curcumene 1,4-Cyclohexadiene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-, (R)- «beta»-Curcumenene
Inchi:	InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6,8-11,13-15H,5,7H2,1-4H
InchiKey:	OFTGWWXCYSXPO-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC(C)=CCCC(C)C1C=CC(C)C=C1
Mol. weight [g/mol]:	204.35
CAS:	28976-67-2

Physical Properties

Property code	Value	Unit	Source
gf	221.31	kJ/mol	Joback Method
hf	-101.24	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	49.34	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.747		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	1513.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1512.00		NIST Webbook

rinpol	1518.00	NIST Webbook
rinpol	1518.00	NIST Webbook
rinpol	1517.00	NIST Webbook
rinpol	1512.00	NIST Webbook
rinpol	1504.00	NIST Webbook
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rinpol	1508.00	NIST Webbook
rinpol	1514.00	NIST Webbook
rinpol	1506.00	NIST Webbook
rinpol	1519.00	NIST Webbook
rinpol	1492.00	NIST Webbook
rinpol	1511.00	NIST Webbook
rinpol	1513.00	NIST Webbook
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rinpol	1516.00	NIST Webbook
rinpol	1507.00	NIST Webbook
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rinpol	1510.00	NIST Webbook
rinpol	1515.00	NIST Webbook
rinpol	1516.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1506.00	NIST Webbook
rinpol	1480.00	NIST Webbook
rinpol	1516.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1516.00	NIST Webbook
rinpol	1493.00	NIST Webbook
rinpol	1512.00	NIST Webbook
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rinpol	1500.00	NIST Webbook
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rinpol	1512.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1509.00	NIST Webbook
rinpol	1516.00	NIST Webbook
ripol	1734.00	NIST Webbook
ripol	1741.00	NIST Webbook
ripol	1741.00	NIST Webbook
ripol	1736.00	NIST Webbook
ripol	1711.00	NIST Webbook

ripol	1744.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1728.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1731.00		NIST Webbook
tb	559.40	K	Joback Method
tc	763.53	K	Joback Method
tf	229.43	K	Joback Method
vc	0.754	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.30	J/mol×K	559.40	Joback Method
cpg	515.63	J/mol×K	593.42	Joback Method
cpg	535.77	J/mol×K	627.44	Joback Method
cpg	554.77	J/mol×K	661.47	Joback Method
cpg	572.67	J/mol×K	695.49	Joback Method
cpg	589.52	J/mol×K	729.51	Joback Method
cpg	605.38	J/mol×K	763.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28976672&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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