

# Benzene, 1-methyl-4-(1,2,2-trimethylcyclopentyl)-, (R)-

**Other names:** Toluene, p-(1,2,2-trimethylcyclopentyl)-, (R)-(+)-

(+)-Cuparene

(R)-Cuparene

Cuparene

Cuparene, (+)-

(R)-(+)-p-(1,2,2-trimethylcyclopentyl)toluene

**Inchi:** InChI=1S/C15H22/c1-12-6-8-13(9-7-12)15(4)11-5-10-14(15,2)3/h6-9H,5,10-11H2,1-4H3

**InchiKey:** SLKPBCXNFNIJSV-HNNXBMFYSA-N

**Formula:** C15H22

**SMILES:** Cc1ccc(C2(C)CCCC2(C)C)cc1

**Mol. weight [g/mol]:** 202.34

**CAS:** 16982-00-6

## Physical Properties

Property code	Value	Unit	Source
gf	196.06	kJ/mol	Joback Method
hf	-57.25	kJ/mol	Joback Method
hfus	10.67	kJ/mol	Joback Method
hvap	49.57	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.463		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1498.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1520.00		NIST Webbook

rinpol	1518.00	NIST Webbook
rinpol	1491.00	NIST Webbook
rinpol	1513.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1509.00	NIST Webbook
rinpol	1515.00	NIST Webbook
rinpol	1488.00	NIST Webbook
rinpol	1488.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1512.10	NIST Webbook
rinpol	1501.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1498.00	NIST Webbook
rinpol	1523.00	NIST Webbook
rinpol	1510.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1516.00	NIST Webbook
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rinpol	1496.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1511.60	NIST Webbook
rinpol	1505.00	NIST Webbook
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rinpol	1504.00	NIST Webbook
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rinpol	1509.00	NIST Webbook
rinpol	1498.00	NIST Webbook
rinpol	1488.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1516.80	NIST Webbook
rinpol	1518.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1501.00	NIST Webbook
rinpol	1506.00	NIST Webbook

ripol	1515.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1508.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1827.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1849.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1825.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1849.00		NIST Webbook
ripol	1849.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1849.00		NIST Webbook
ripol	1849.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1826.00		NIST Webbook
ripol	1803.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1825.00		NIST Webbook
ripol	1776.00		NIST Webbook
ripol	1825.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1804.00		NIST Webbook
ripol	1811.00		NIST Webbook
ripol	1838.00		NIST Webbook
tb	585.35	K	Joback Method
tc	824.05	K	Joback Method
tf	352.21	K	Joback Method
vc	0.704	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	480.48	J/mol×K	585.35	Joback Method
cpg	501.95	J/mol×K	625.13	Joback Method
cpg	522.02	J/mol×K	664.92	Joback Method
cpg	541.00	J/mol×K	704.70	Joback Method
cpg	559.17	J/mol×K	744.48	Joback Method
cpg	576.82	J/mol×K	784.27	Joback Method
cpg	594.26	J/mol×K	824.05	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C16982006&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16982006&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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