# Longifolene

| | |
|---|---|
| **Other names:** | (+)-Longifolen |
| | (+)-Longifolene |
| | (-)-isolongifolene |
| | (2S,4aR)-1,1,5,5-tetramethyl-1,3,4,5,6,7-hexahydro-2H-2,4a-methanonaphthalene |
| | (2S,4aR)-1,3,4,5,6,7-hexahydro-1,1,5,5-tetramethyl-2H-2,4a-methanonaphthalene |
| | 1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene- |
| | 1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene-, (1S,3aR,4S,8aS)- |
| | 1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene-, (1S,3aR,4S,8aS)-(+)- |
| | 1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene-, [1S-(1«alpha»,3a«beta»,4«alpha»,8a«beta»)]- |
| | D-longifolene |
| | Junipen |
| | Junipene |
| | Kuromatsuen |
| | Kuromatsuene |
| | Longifolen |
| | Longifolene (=Junipene) |
| | [1S-(1«alpha»,3a«beta»,4«alpha»,8a«beta»)]-decahydro-4,8,8-trimethyl-9-methylene-1,4 |
| | «alpha»-Longifolene |
| **Inchi:** | InChI=1S/C15H24/c1-10-11-6-7-12-13(11)14(2,3)8-5-9-15(10,12)4/h11-13H,1,5-9H2,2-4H |
| **InchiKey:** | PDSNLYSELAIEBU-UHFFFAOYSA-N |
| **Formula:** | C15H24 |
| **SMILES:** | C=C1C2CCC3C2C(C)(C)CCCC13C |
| **Mol. weight [g/mol]:** | 204.35 |
| **CAS:** | 475-20-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 260.15 | kJ/mol | Joback Method |
| hf | -72.81 | kJ/mol | Joback Method |
| hfus | 13.20 | kJ/mol | Joback Method |
| hvap | 46.31 | kJ/mol | Joback Method |
| log10ws | -4.43 | | Crippen Method |
| logp | 4.415 | | Crippen Method |
| mcvol | 185.330 | ml/mol | McGowan Method |
| pc | 2113.89 | kPa | Joback Method |
| rinpol | 1400.00 | | NIST Webbook |
| rinpol | 1427.00 | | NIST Webbook |

| | | |
|---|---|---|
| rinpol | 1440.00 | NIST Webbook |
| rinpol | 1404.00 | NIST Webbook |
| rinpol | 1403.00 | NIST Webbook |
| rinpol | 1398.00 | NIST Webbook |
| rinpol | 1408.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1415.70 | NIST Webbook |
| rinpol | 1448.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1399.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1418.00 | NIST Webbook |
| rinpol | 1427.00 | NIST Webbook |
| rinpol | 1395.00 | NIST Webbook |
| rinpol | 1380.00 | NIST Webbook |
| rinpol | 1405.00 | NIST Webbook |
| rinpol | 1404.00 | NIST Webbook |
| rinpol | 1386.00 | NIST Webbook |
| rinpol | 1450.00 | NIST Webbook |
| rinpol | 1412.00 | NIST Webbook |
| rinpol | 1387.00 | NIST Webbook |
| rinpol | 1405.00 | NIST Webbook |
| rinpol | 1432.00 | NIST Webbook |
| rinpol | 1417.00 | NIST Webbook |
| rinpol | 1407.60 | NIST Webbook |
| rinpol | 1409.10 | NIST Webbook |
| rinpol | 1412.60 | NIST Webbook |
| rinpol | 1400.00 | NIST Webbook |
| rinpol | 1409.00 | NIST Webbook |
| rinpol | 1409.00 | NIST Webbook |
| rinpol | 1408.00 | NIST Webbook |
| rinpol | 1407.00 | NIST Webbook |
| rinpol | 1414.00 | NIST Webbook |
| rinpol | 1389.00 | NIST Webbook |
| rinpol | 1415.00 | NIST Webbook |
| rinpol | 1404.00 | NIST Webbook |
| rinpol | 1404.00 | NIST Webbook |
| rinpol | 1416.00 | NIST Webbook |
| rinpol | 1404.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1441.00 | NIST Webbook |
| rinpol | 1406.00 | NIST Webbook |
| rinpol | 1418.00 | NIST Webbook |

| | | |
|---|---|---|
| rinpol | 1388.00 | NIST Webbook |
| rinpol | 1413.40 | NIST Webbook |
| rinpol | 1398.00 | NIST Webbook |
| rinpol | 1406.30 | NIST Webbook |
| rinpol | 1389.60 | NIST Webbook |
| rinpol | 1398.00 | NIST Webbook |
| rinpol | 1414.00 | NIST Webbook |
| rinpol | 1404.00 | NIST Webbook |
| rinpol | 1411.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1408.00 | NIST Webbook |
| rinpol | 1430.00 | NIST Webbook |
| rinpol | 1406.00 | NIST Webbook |
| rinpol | 1409.00 | NIST Webbook |
| rinpol | 1397.00 | NIST Webbook |
| rinpol | 1401.00 | NIST Webbook |
| rinpol | 1409.00 | NIST Webbook |
| rinpol | 1403.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1405.00 | NIST Webbook |
| rinpol | 1400.00 | NIST Webbook |
| rinpol | 1415.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1398.00 | NIST Webbook |
| rinpol | 1400.00 | NIST Webbook |
| rinpol | 1395.00 | NIST Webbook |
| rinpol | 1406.00 | NIST Webbook |
| rinpol | 1398.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1418.00 | NIST Webbook |
| rinpol | 1444.00 | NIST Webbook |
| rinpol | 1437.00 | NIST Webbook |
| rinpol | 1416.00 | NIST Webbook |
| rinpol | 1386.00 | NIST Webbook |
| rinpol | 1410.00 | NIST Webbook |
| rinpol | 1393.00 | NIST Webbook |
| rinpol | 1388.00 | NIST Webbook |
| rinpol | 1404.00 | NIST Webbook |
| rinpol | 1400.00 | NIST Webbook |
| rinpol | 1399.00 | NIST Webbook |
| rinpol | 1393.00 | NIST Webbook |
| rinpol | 1380.00 | NIST Webbook |
| rinpol | 1397.00 | NIST Webbook |

| | | |
|---|---|---|
| rinpol | 1401.00 | NIST Webbook |
| rinpol | 1387.00 | NIST Webbook |
| rinpol | 1401.00 | NIST Webbook |
| rinpol | 1434.00 | NIST Webbook |
| rinpol | 1408.00 | NIST Webbook |
| rinpol | 1398.00 | NIST Webbook |
| rinpol | 1388.00 | NIST Webbook |
| rinpol | 1398.00 | NIST Webbook |
| rinpol | 1413.00 | NIST Webbook |
| rinpol | 1396.00 | NIST Webbook |
| rinpol | 1380.00 | NIST Webbook |
| rinpol | 1400.00 | NIST Webbook |
| rinpol | 1401.00 | NIST Webbook |
| rinpol | 1398.00 | NIST Webbook |
| rinpol | 1398.00 | NIST Webbook |
| rinpol | 1420.00 | NIST Webbook |
| rinpol | 1412.00 | NIST Webbook |
| rinpol | 1424.00 | NIST Webbook |
| rinpol | 1404.00 | NIST Webbook |
| rinpol | 1398.00 | NIST Webbook |
| rinpol | 1409.00 | NIST Webbook |
| rinpol | 1418.00 | NIST Webbook |
| rinpol | 1405.00 | NIST Webbook |
| rinpol | 1407.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1388.00 | NIST Webbook |
| rinpol | 1411.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |
| rinpol | 1438.00 | NIST Webbook |
| rinpol | 1451.00 | NIST Webbook |
| rinpol | 1455.00 | NIST Webbook |
| rinpol | 1408.00 | NIST Webbook |
| rinpol | 1407.00 | NIST Webbook |
| rinpol | 1447.00 | NIST Webbook |
| rinpol | 1405.00 | NIST Webbook |
| rinpol | 1408.00 | NIST Webbook |
| rinpol | 1408.00 | NIST Webbook |
| rinpol | 1389.00 | NIST Webbook |
| rinpol | 1408.00 | NIST Webbook |
| rinpol | 1384.00 | NIST Webbook |
| rinpol | 1416.00 | NIST Webbook |
| rinpol | 1400.00 | NIST Webbook |
| rinpol | 1423.00 | NIST Webbook |
| rinpol | 1402.00 | NIST Webbook |

| | | | |
|---|---|---|---|
| rinpol | 1409.00 | | NIST Webbook |
| rinpol | 1413.00 | | NIST Webbook |
| rinpol | 1409.00 | | NIST Webbook |
| ripol | 1622.00 | | NIST Webbook |
| ripol | 1622.00 | | NIST Webbook |
| ripol | 1620.00 | | NIST Webbook |
| ripol | 1619.00 | | NIST Webbook |
| ripol | 1600.00 | | NIST Webbook |
| ripol | 1600.00 | | NIST Webbook |
| ripol | 1590.00 | | NIST Webbook |
| ripol | 1587.00 | | NIST Webbook |
| ripol | 1590.00 | | NIST Webbook |
| ripol | 1583.00 | | NIST Webbook |
| ripol | 1577.00 | | NIST Webbook |
| ripol | 1569.00 | | NIST Webbook |
| ripol | 1562.00 | | NIST Webbook |
| ripol | 1557.00 | | NIST Webbook |
| ripol | 1574.00 | | NIST Webbook |
| ripol | 1580.00 | | NIST Webbook |
| ripol | 1574.00 | | NIST Webbook |
| ripol | 1608.00 | | NIST Webbook |
| ripol | 1575.00 | | NIST Webbook |
| ripol | 1568.00 | | NIST Webbook |
| ripol | 1576.00 | | NIST Webbook |
| ripol | 1587.00 | | NIST Webbook |
| ripol | 1565.00 | | NIST Webbook |
| ripol | 1577.00 | | NIST Webbook |
| ripol | 1566.00 | | NIST Webbook |
| ripol | 1577.00 | | NIST Webbook |
| ripol | 1577.00 | | NIST Webbook |
| ripol | 1576.00 | | NIST Webbook |
| ripol | 1583.00 | | NIST Webbook |
| ripol | 1574.00 | | NIST Webbook |
| ripol | 1570.00 | | NIST Webbook |
| ripol | 1574.00 | | NIST Webbook |
| ripol | 1574.00 | | NIST Webbook |
| ripol | 1595.00 | | NIST Webbook |
| ripol | 1565.00 | | NIST Webbook |
| ripol | 1623.00 | | NIST Webbook |
| ripol | 1568.00 | | NIST Webbook |
| ripol | 1583.00 | | NIST Webbook |
| ripol | 1574.00 | | NIST Webbook |
| tb | 561.66 | K | Joback Method |
| tc | 785.91 | K | Joback Method |

| | | | |
|---|---|---|---|
| tf | 358.59 | K | Joback Method |
| vc | 0.709 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 501.94 | J/mol×K | 561.66 | Joback Method |
| cpg | 525.20 | J/mol×K | 599.03 | Joback Method |
| cpg | 546.85 | J/mol×K | 636.41 | Joback Method |
| cpg | 567.18 | J/mol×K | 673.78 | Joback Method |
| cpg | 586.48 | J/mol×K | 711.16 | Joback Method |
| cpg | 605.02 | J/mol×K | 748.53 | Joback Method |
| cpg | 623.10 | J/mol×K | 785.91 | Joback Method |
| hvapt | 62.60 | kJ/mol | 298.15 | Vapor pressure and vaporization enthalpy studies of (+)-longifolene, (-)-isolongifolene and beta-myrcene by correlation gas chromatography |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 528.20 | K | 94.10 | NIST Webbook |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Vapor pressure and vaporization enthalpy studies of (+)-longifolene, (-)-isolongifolene and beta-myrcene by correlation gas chromatography:** https://www.doi.org/10.1016/j.jct.2018.12.013

**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=C475207&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |