# MEGASTIGMA-4,6(Z),8(E)-TRIENE

**Other names:** Cyclohexene, 6-(2-butenylidene)-1,5,5-trimethyl-, (Z,E)-
Cyclohexene, 6-(2E)-2-buten-1-ylidene-1,5,5-trimethyl-, (6Z)-
**Inchi:** InChI=1S/C13H20/c1-5-6-9-12-11(2)8-7-10-13(12,3)4/h5-6,8-9H,7,10H2,1-4H3/b6-5+,12
**InchiKey:** BYDQKMZEOZVIJM-HFACTSAFSA-N
**Formula:** C13H20
**SMILES:** C/C=C/C=C1\C(C)=CCCC1(C)C
**Mol. weight [g/mol]:** 176.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 47.69 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 16.32 | kJ/mol | Joback Method |
| logp | 4.255 | | Crippen Method |
| mcvol | 170.270 | ml/mol | McGowan Method |
| rinpol | 1329.00 | | NIST Webbook |
| rinpol | 1351.00 | | NIST Webbook |
| rinpol | 1373.00 | | NIST Webbook |
| ripol | 2323.00 | | NIST Webbook |
| ripol | 2323.00 | | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 394.30 | J/mol×K | 531.57 | Joback Method |
| cpg | 413.03 | J/mol×K | 567.71 | Joback Method |
| cpg | 430.58 | J/mol×K | 603.85 | Joback Method |
| cpg | 447.07 | J/mol×K | 639.99 | Joback Method |
| cpg | 462.65 | J/mol×K | 676.13 | Joback Method |
| cpg | 477.45 | J/mol×K | 712.27 | Joback Method |
| cpg | 491.60 | J/mol×K | 748.41 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C51468850&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |