# 2-{(4E)-3,6-dimethyl-6-[3-(3,3,4-trimethylcyclohex
# Isomer # 1

**Inchi:** InChI=1S/C33H56/c1-12-33(11,22-20-25(3)29-17-16-27(5)31(7,8)23-29)21-19-24(2)13-1
**InchiKey:** VIBZFVIDYOALBH-NMKLIDAOSA-N
**Formula:** C33H56
**SMILES:** C=CC(C)(C=CC(C)CCC1C(=C)CCC(C)C1(C)C)CCC(C)=C1CCC(C)C(C)(C)C1
**Mol. weight [g/mol]:** 452.80

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 500.22 | kJ/mol | Joback Method |
| hf | -267.25 | kJ/mol | Joback Method |
| hfus | 41.35 | kJ/mol | Joback Method |
| hvap | 85.31 | kJ/mol | Joback Method |
| log10ws | -11.15 | | Crippen Method |
| logp | 10.723 | | Crippen Method |
| mcvol | 436.910 | ml/mol | McGowan Method |
| pc | 688.53 | kPa | Joback Method |
| rinpol | 2766.00 | | NIST Webbook |
| tb | 982.86 | K | Joback Method |
| tc | 1208.68 | K | Joback Method |
| tf | 502.17 | K | Joback Method |
| vc | 1.655 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1587.87 | J/mol×K | 982.86 | Joback Method |
| cpg | 1621.95 | J/mol×K | 1020.50 | Joback Method |
| cpg | 1656.41 | J/mol×K | 1058.13 | Joback Method |
| cpg | 1691.58 | J/mol×K | 1095.77 | Joback Method |
| cpg | 1727.79 | J/mol×K | 1133.40 | Joback Method |
| cpg | 1765.37 | J/mol×K | 1171.04 | Joback Method |
| cpg | 1804.64 | J/mol×K | 1208.68 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R586446&Units=SI |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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