# 3-(1-adamantyl)pentene-2

**Inchi:** InChI=1S/C15H24/c1-3-14(4-2)15-8-11-5-12(9-15)7-13(6-11)10-15/h3,11-13H,4-10H2,1-
**InchiKey:** IWINQLXEHRHZRS-BNNQUZSASA-N
**Formula:** C15H24
**SMILES:** CC=C(CC)C12CC3CC(CC(C3)C1)C2
**Mol. weight [g/mol]:** 204.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 304.04 | kJ/mol | Joback Method |
| hf | -38.36 | kJ/mol | Joback Method |
| hfus | 20.58 | kJ/mol | Joback Method |
| hvap | 47.47 | kJ/mol | Joback Method |
| log10ws | -4.67 | | Crippen Method |
| logp | 4.559 | | Crippen Method |
| mcvol | 185.330 | ml/mol | McGowan Method |
| pc | 2115.83 | kPa | Joback Method |
| rinpol | 1559.00 | | NIST Webbook |
| rinpol | 1571.00 | | NIST Webbook |
| rinpol | 1587.00 | | NIST Webbook |
| rinpol | 1559.00 | | NIST Webbook |
| rinpol | 1600.00 | | NIST Webbook |
| ripol | 1811.00 | | NIST Webbook |
| ripol | 1834.00 | | NIST Webbook |
| ripol | 1854.00 | | NIST Webbook |
| ripol | 1811.00 | | NIST Webbook |
| tb | 566.70 | K | Joback Method |
| tc | 786.31 | K | Joback Method |
| tf | 309.73 | K | Joback Method |
| vc | 0.717 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 502.70 | J/mol×K | 566.70 | Joback Method |

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|---|---|---|---|---|
| cpg | 525.66 | J/mol×K | 603.30 | Joback Method |
| cpg | 547.01 | J/mol×K | 639.90 | Joback Method |
| cpg | 566.95 | J/mol×K | 676.51 | Joback Method |
| cpg | 585.72 | J/mol×K | 713.11 | Joback Method |
| cpg | 603.54 | J/mol×K | 749.71 | Joback Method |
| cpg | 620.62 | J/mol×K | 786.31 | Joback Method |

# Sources

| | |
|---|---|
| **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=R304640&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |