# petasitene

**Inchi:** InChI=1S/C15H24/c1-10(2)13-7-8-14(3)11-5-6-12(9-11)15(13,14)4/h7,10-12H,5-6,8-9H2
**InchiKey:** ZGKPBXWQOYDEMA-UHFFFAOYSA-N
**Formula:** C15H24
**SMILES:** CC(C)C1=CCC2(C)C3CCC(C3)C12C
**Mol. weight [g/mol]:** 204.35
**CAS:** 443124-67-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 244.77 | kJ/mol | Joback Method |
| hf | -89.52 | kJ/mol | Joback Method |
| hfus | 12.70 | kJ/mol | Joback Method |
| hvap | 46.85 | kJ/mol | Joback Method |
| log10ws | -4.43 | | Crippen Method |
| logp | 4.415 | | Crippen Method |
| mcvol | 185.330 | ml/mol | McGowan Method |
| pc | 2149.31 | kPa | Joback Method |
| rinpol | 1400.00 | | NIST Webbook |
| rinpol | 1385.00 | | NIST Webbook |
| rinpol | 1400.00 | | NIST Webbook |
| rinpol | 1404.60 | | NIST Webbook |
| tb | 566.60 | K | Joback Method |
| tc | 789.18 | K | Joback Method |
| tf | 350.95 | K | Joback Method |
| vc | 0.714 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 501.59 | J/mol×K | 566.60 | Joback Method |
| cpg | 523.50 | J/mol×K | 603.70 | Joback Method |
| cpg | 543.86 | J/mol×K | 640.79 | Joback Method |
| cpg | 562.98 | J/mol×K | 677.89 | Joback Method |
| cpg | 581.15 | J/mol×K | 714.99 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 598.68 | J/mol×K | 752.08 | Joback Method |
| cpg | 615.88 | J/mol×K | 789.18 | Joback Method |

# Sources

| | |
|---|---|
| **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=C443124672&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 |
| **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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