

Seychellene

| | |
|-----------------------------|--|
| Other names: | 1,6-Methanonaphthalene, decahydro-1,4,8a-trimethyl-9-methylene-, (1S,4S,4aS,6R,8aS)-(-)- |
| Inchi: | 1,6-Methanonaphthalene, decahydro-1,4,8a-trimethyl-9-methylene-, *1S:(1«alpha»,4«alpha»,4a«beta»,6«alpha» |
| InchiKey: | InChI=1S/C15H24/c1-10-5-7-14(3)11(2)12-6-8-15(14,4)13(10)9-12/h10,12-13H,2,5-9H2, |
| InchiKey: | QQWUXXGYAQM-TAT-UHFFFAOYSA-N |
| Formula: | C15H24 |
| SMILES: | C=C1C2CCC3(C)C(C2)C(C)CCC13C |
| Mol. weight [g/mol]: | 204.35 |
| CAS: | 20085-93-2 |

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 | 1460.00 | | NIST Webbook |
| rinpol | 1459.00 | | NIST Webbook |
| rinpol | 1464.00 | | NIST Webbook |
| rinpol | 1448.00 | | NIST Webbook |
| rinpol | 1461.00 | | NIST Webbook |
| rinpol | 1460.00 | | NIST Webbook |
| rinpol | 1456.00 | | NIST Webbook |
| rinpol | 1456.00 | | NIST Webbook |
| rinpol | 1460.00 | | NIST Webbook |
| rinpol | 1460.00 | | NIST Webbook |
| rinpol | 1458.00 | | NIST Webbook |
| rinpol | 1459.00 | | NIST Webbook |
| rinpol | 1460.00 | | NIST Webbook |
| rinpol | 1451.80 | | NIST Webbook |
| rinpol | 1461.00 | | NIST Webbook |
| rinpol | 1457.00 | | NIST Webbook |
| ripol | 1669.00 | | NIST Webbook |
| ripol | 1669.00 | | NIST Webbook |

| | | | |
|----|--------|----------------------|---------------|
| tb | 561.66 | K | Joback Method |
| tc | 785.91 | K | Joback Method |
| tf | 358.59 | K | Joback Method |
| vc | 0.709 | m ³ /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 |

Sources

| | |
|------------------------|---|
| 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=C20085932&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |

Latest version available from:

<https://www.cheméo.com/cid/79-074-3/Seychellene.pdf>

Generated by Cheméo on 2024-04-30 06:34:14.72608064 +0000 UTC m=+16748103.646657951.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.