

Bicyclo[2.2.1]heptane, 1,7,7-trimethyl-

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| Other names: | Bornane Bornylane Camphane 1,7,7-Trimethylbicyclo[2.2.1]heptane |
| Inchi: | InChI=1S/C10H18/c1-9(2)8-4-6-10(9,3)7-5-8/h8H,4-7H2,1-3H3 |
| InchiKey: | BEWYHVAWEKZDPP-UHFFFAOYSA-N |
| Formula: | C10H18 |
| SMILES: | CC12CCC(CC1)C2(C)C |
| Mol. weight [g/mol]: | 138.25 |
| CAS: | 464-15-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|----------------------|----------------|
| gf | 124.03 | kJ/mol | Joback Method |
| hf | -100.15 | kJ/mol | Joback Method |
| hfus | 4.30 | kJ/mol | Joback Method |
| hvap | 35.24 | kJ/mol | Joback Method |
| log10ws | -3.07 | | Crippen Method |
| logp | 3.223 | | Crippen Method |
| mcvol | 130.040 | ml/mol | McGowan Method |
| pc | 2966.57 | kPa | Joback Method |
| rinpola | 980.00 | | NIST Webbook |
| ripola | 1140.00 | | NIST Webbook |
| ripola | 1140.00 | | NIST Webbook |
| ripola | 1131.00 | | NIST Webbook |
| ripola | 1144.00 | | NIST Webbook |
| tb | 441.76 | K | Joback Method |
| tc | 656.69 | K | Joback Method |
| tf | 431.00 ± 5.00 | K | NIST Webbook |
| tf | 429.40 ± 2.00 | K | NIST Webbook |
| vc | 0.496 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 288.12 | J/mol×K | 441.76 | Joback Method |
| cpg | 308.54 | J/mol×K | 477.58 | Joback Method |
| cpg | 327.12 | J/mol×K | 513.40 | Joback Method |
| cpg | 344.11 | J/mol×K | 549.22 | Joback Method |
| cpg | 359.72 | J/mol×K | 585.04 | Joback Method |
| cpg | 374.21 | J/mol×K | 620.87 | Joback Method |
| cpg | 387.79 | J/mol×K | 656.69 | 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=C464153&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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 |
| hvac: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccol: | 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.chemeo.com/cid/76-725-3/Bicyclo-2-2-1-heptane-1-7-7-trimethyl.pdf>

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