# Pseudoephedrine

| | |
|---|---|
| **Other names:** | Pseudoephedrine, (+)- |
| | Benzenemethanol, «alpha»-[1-(methylamino)ethyl]-, [S-(R*,R*)]- |
| | «psi»-Ephedrine |
| | «psi»-Ephedrine, (+)- |
| | «psi»-Ephedrin |
| | (+)-Pseudoephedrine |
| | D-«psi»-Ephedrine |
| | D-isoephedrine |
| | D-pseudoephedrine |
| | trans-Ephedrine |
| | Isoephedrine |
| | L-(+)-Pseudoephedrine |
| | Sudafed |
| | Pseudoephedrine, L-(+)- |
| | Besan |
| | d-psi-Ephedrine |
| | psi-Ephedrine |
| | «alpha»-((1S)-1-(Methylamino)ethyl)benzyl alcohol, («alpha»S)- |
| | d-psi-2-Methylamino-1-phenyl-1-propanol |
| | [S-(R*,R*)]-«alpha»-[1-(methylamino)ethyl]benzenemethanol |
| | «alpha»-[(1S)-1-(Methylamino)ethyl]benzenemethanol, («alpha»S)- |
| | Pseudoephedrine d-form |
| | (+)-(1S,2S)-Pseudoephedrine |
| | (+)-threo-Ephedrine |
| | (1S,2S)-(+)-Pseudoephedrine |
| | (1S,2S)-Pseudoephedrine |
| | L(+)-«psi»-Ephedrine |
| | (+) threo-2-(methylamino)-1-phenyl-1-propanol (pseudoephedrine) |
| **Inchi:** | InChI=1S/C10H15NO/c1-8(11-2)10(12)9-6-4-3-5-7-9/h3-8,10-12H,1-2H3/t8-,10-/m0/s1 |
| **InchiKey:** | KWGRBVOPPLSCSI-WPRPVWTQSA-N |
| **Formula:** | C10H15NO |
| **SMILES:** | CNC(C)C(O)c1ccccc1 |
| **Mol. weight [g/mol]:** | 165.23 |
| **CAS:** | 90-82-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|

| | | | |
|---|---|---|---|
| gf | 93.42 | kJ/mol | Joback Method |
| hf | -122.52 | kJ/mol | Joback Method |
| hfus | 17.84 | kJ/mol | Joback Method |
| hvap | 62.47 | kJ/mol | Joback Method |
| log10ws | -2.13 | | Crippen Method |
| logp | 1.328 | | Crippen Method |
| mcvol | 143.850 | ml/mol | McGowan Method |
| pc | 3356.75 | kPa | Joback Method |
| rinpol | 1357.00 | | NIST Webbook |
| rinpol | 1400.00 | | NIST Webbook |
| rinpol | 1360.00 | | NIST Webbook |
| rinpol | 1376.00 | | NIST Webbook |
| rinpol | 1360.00 | | NIST Webbook |
| rinpol | 1360.00 | | NIST Webbook |
| rinpol | 1350.00 | | NIST Webbook |
| rinpol | 1350.00 | | NIST Webbook |
| rinpol | 1357.00 | | NIST Webbook |
| rinpol | 1362.00 | | NIST Webbook |
| rinpol | 1367.00 | | NIST Webbook |
| rinpol | 1397.00 | | NIST Webbook |
| rinpol | 1350.00 | | NIST Webbook |
| rinpol | 1400.00 | | NIST Webbook |
| rinpol | 1354.00 | | NIST Webbook |
| rinpol | 1360.00 | | NIST Webbook |
| rinpol | 1350.00 | | NIST Webbook |
| rinpol | 1350.00 | | NIST Webbook |
| rinpol | 1354.00 | | NIST Webbook |
| rinpol | 1360.00 | | NIST Webbook |
| rinpol | 1376.00 | | NIST Webbook |
| rinpol | 1398.00 | | NIST Webbook |
| ripol | 2217.00 | | NIST Webbook |
| ripol | 2225.00 | | NIST Webbook |
| ripol | 2185.00 | | NIST Webbook |
| ripol | 2195.00 | | NIST Webbook |
| ripol | 2205.00 | | NIST Webbook |
| ripol | 2213.00 | | NIST Webbook |
| tb | 596.35 | K | Joback Method |
| tc | 797.42 | K | Joback Method |
| tf | 312.36 | K | Joback Method |
| vc | 0.529 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 361.03 | J/mol×K | 596.35 | Joback Method |
| cpg | 374.04 | J/mol×K | 629.86 | Joback Method |
| cpg | 386.27 | J/mol×K | 663.37 | Joback Method |
| cpg | 397.75 | J/mol×K | 696.89 | Joback Method |
| cpg | 408.51 | J/mol×K | 730.40 | Joback Method |
| cpg | 418.60 | J/mol×K | 763.91 | Joback Method |
| cpg | 428.04 | J/mol×K | 797.42 | Joback Method |
| hfust | 31.95 | kJ/mol | 392.40 | NIST Webbook |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C90824&Units=SI
**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

# 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
**hfust:** Enthalpy of fusion at a given temperature
**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

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