# Amitriptyline

**Other names:**

1-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-
10,11-Dihydro-5-(«gamma»-dimethylaminopropylidene)-5H-dibenzo(a,d)cycloheptene
10,11-Dihydro-5-(Â«gammaÂ»-dimethylaminopropylidene)-5H-dibenzo(a,d)cycloheptene
10,11-Dihydro-N,N-dimethyl-5H-dibenzo(a,d)heptalene-«DELTA»5,«gamma»-propylamin
10,11-Dihydro-N,N-dimethyl-5H-dibenzo(a,d)heptalene-Â«DELTAÂ»5,Â«gammaÂ»-prop
3-(10,11-Dihydro-5H-dibenzo(a,d)cyclohepten-5-ylidene)-N,N-dimethyl-1-propanamine
5-(3'-Dimethylaminopropylidene)-dibenzo-(a,d)(1,4)-cycloheptadiene
5-(3-Dimethylaminopropylidene)-10,11-dihydro-5H-dibenzo(a,d)cycloheptene
5-(«gamma»-Dimethylaminopropylidene)-10,11-dihydro-5H-dibenzo(a,d)cycloheptene
5-(«gamma»-Dimethylaminopropylidene)-5H-Dibenzo[a,d][1,4]cycloheptadiene
5-(«gamma»-Dimethylaminopropylidene)-5H-dibenzo(a,d)-10,11-dihydrocycloheptene
5-(«gamma»-Dimethylaminopropylidine)-5H-dibenzo(a,d)(1,4)cycloheptadiene
5-(Â«gammaÂ»-Dimethylaminopropylidene)-10,11-dihydro-5H-dibenzo(a,d)cycloheptene
5-(Â«gammaÂ»-Dimethylaminopropylidene)-5H-Dibenzo[a,d][1,4]cycloheptadiene
5-(Â«gammaÂ»-Dimethylaminopropylidene)-5H-dibenzo(a,d)-10,11-dihydrocycloheptene
5-(Â«gammaÂ»-Dimethylaminopropylidine)-5H-dibenzo(a,d)(1,4)cycloheptadiene
5H-Dibenzo[a,d]cycloheptene-«DELTA»5,«gamma»-propylamine, 10,11-dihydro-N,N-dimethyl-
5H-Dibenzo[a,d]cycloheptene-Â«DELTAÂ»5,Â«gammaÂ»-propylamine, 10,11-dihydro-N,N-dimethyl-
Adepress
Adepril
Amitriptylin
Amitryptiline
Damilan
Damilen
Damitriptyline
Elanil
Elavil
Flavyl
Lantron
Proheptadiene
Ro 4-1575
Seroten
Triptanol
Triptisol
Tryptanol

**Inchi:** InChI=1S/C20H23N/c1-21(2)15-7-12-20-18-10-5-3-8-16(18)13-14-17-9-4-6-11-19(17)20/

**InchiKey:** KRMDCWKBEZIMAB-UHFFFAOYSA-N

**Formula:** C20H23N

**SMILES:** CN(C)CCC=C1c2ccccc2CCc2ccccc21

**Mol. weight [g/mol]:** 277.40

**CAS:** 50-48-6

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 547.78 | kJ/mol | Joback Method |
| hf | 230.69 | kJ/mol | Joback Method |
| hfus | 35.27 | kJ/mol | Joback Method |
| hvap | 69.04 | kJ/mol | Joback Method |
| ie | 8.32 ± 0.08 | eV | NIST Webbook |
| ie | 8.26 ± 0.07 | eV | NIST Webbook |
| log10ws | -4.46 | | Aqueous and cosolvent solubility data for drug-like organic compounds |
| log10ws | -4.55 | | Aqueous Solubility Prediction Method |
| logp | 4.169 | | Crippen Method |
| mcvol | 239.960 | ml/mol | McGowan Method |
| pc | 1864.33 | kPa | Joback Method |
| rinpol | 2179.00 | | NIST Webbook |
| rinpol | 2204.00 | | NIST Webbook |
| rinpol | 2162.00 | | NIST Webbook |
| rinpol | 2196.00 | | NIST Webbook |
| rinpol | 2200.00 | | NIST Webbook |
| rinpol | 2200.00 | | NIST Webbook |
| rinpol | 2182.00 | | NIST Webbook |
| rinpol | 2194.00 | | NIST Webbook |
| rinpol | 2188.00 | | NIST Webbook |
| rinpol | 2201.00 | | NIST Webbook |
| rinpol | 2236.00 | | NIST Webbook |
| rinpol | 2185.00 | | NIST Webbook |
| rinpol | 2195.00 | | NIST Webbook |
| rinpol | 2220.00 | | NIST Webbook |
| rinpol | 2200.00 | | NIST Webbook |
| rinpol | 2252.00 | | NIST Webbook |
| rinpol | 2194.00 | | NIST Webbook |
| rinpol | 2179.00 | | NIST Webbook |
| rinpol | 2220.00 | | NIST Webbook |
| rinpol | 2187.00 | | NIST Webbook |
| rinpol | 2192.00 | | NIST Webbook |
| rinpol | 2169.00 | | NIST Webbook |
| rinpol | 2162.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 2190.00 | | NIST Webbook |
| rinpol | 2208.00 | | NIST Webbook |
| rinpol | 2181.00 | | NIST Webbook |
| rinpol | 2208.00 | | NIST Webbook |
| rinpol | 2196.00 | | NIST Webbook |
| rinpol | 2166.00 | | NIST Webbook |
| rinpol | 2191.00 | | NIST Webbook |
| rinpol | 2200.00 | | NIST Webbook |
| rinpol | 2209.00 | | NIST Webbook |
| rinpol | 2174.00 | | NIST Webbook |
| rinpol | 2181.00 | | NIST Webbook |
| rinpol | 2162.00 | | NIST Webbook |
| rinpol | 2179.00 | | NIST Webbook |
| rinpol | 2210.00 | | NIST Webbook |
| rinpol | 2210.00 | | NIST Webbook |
| rinpol | 2190.00 | | NIST Webbook |
| rinpol | 2190.00 | | NIST Webbook |
| rinpol | 2181.00 | | NIST Webbook |
| rinpol | 2208.00 | | NIST Webbook |
| ripol | 2924.00 | | NIST Webbook |
| ripol | 2924.00 | | NIST Webbook |
| tb | 750.81 | K | Joback Method |
| tc | 982.62 | K | Joback Method |
| tf | 387.65 | K | Aqueous Solubility Prediction Method |
| vc | 0.898 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 685.45 | J/mol×K | 750.81 | Joback Method |
| cpg | 703.74 | J/mol×K | 789.44 | Joback Method |
| cpg | 720.79 | J/mol×K | 828.08 | Joback Method |
| cpg | 736.74 | J/mol×K | 866.71 | Joback Method |
| cpg | 751.71 | J/mol×K | 905.35 | Joback Method |
| cpg | 765.85 | J/mol×K | 943.98 | Joback Method |
| cpg | 779.29 | J/mol×K | 982.62 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Aqueous and cosolvent solubility data for drug-like organic compounds:** | https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/ |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C50486&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 |
| **ie:** | Ionization energy |
| **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 |