

# Maprotiline M(HO-propyl), acetylated

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C24H27NO3/c1-16(26)25(3)15-18(28-17(2)27)14-24-13-12-19(20-8-4-6-10-22) |
| <b>InchiKey:</b>            | GNFRHRIWAOEYML-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C24H27NO3  |
| <b>SMILES:</b>              | CC(=O)OC(CN(C)C(C)=O)CC12CCC(c3ccccc31)c1ccccc12                                 |
| <b>Mol. weight [g/mol]:</b> | 377.48   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 242.47  | kJ/mol               | Joback Method  |
| hf            | -210.54 | kJ/mol               | Joback Method  |
| hfus          | 43.28   | kJ/mol               | Joback Method  |
| hvap          | 90.78   | kJ/mol               | Joback Method  |
| log10ws       | -4.96   |                      | Crippen Method |
| logp          | 4.012   |                      | Crippen Method |
| mvol          | 298.770 | ml/mol               | McGowan Method |
| pc            | 1574.70 | kPa                  | Joback Method  |
| rinpol        | 2426.00 |                      | NIST Webbook   |
| tb            | 959.18  | K                    | Joback Method  |
| tc            | 1194.36 | K                    | Joback Method  |
| tf            | 644.50  | K                    | Joback Method  |
| vc            | 1.133   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 991.20  | J/molxK | 959.18          | Joback Method |
| cpg           | 1011.87 | J/molxK | 998.38          | Joback Method |
| cpg           | 1032.97 | J/molxK | 1037.57         | Joback Method |
| cpg           | 1054.78 | J/molxK | 1076.77         | Joback Method |
| cpg           | 1077.61 | J/molxK | 1115.96         | Joback Method |
| cpg           | 1101.73 | J/molxK | 1155.16         | Joback Method |
| cpg           | 1127.44 | J/molxK | 1194.36         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R311009&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R311009&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mccvol:</b>  | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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