# Formetanate

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|---|---|
| **Other names:** | 3-([(Dimethylamino)methylidene]amino)phenyl methylcarbamate<br>3-[(Dimethylamino)methylenimino]phenyl N-methylcarbamate<br>Carbamic acid, methyl-, ester with N'-(m-hydroxyphenyl)-N,N-dimethylformamidine<br>Carbamic acid, methyl-, m-(((dimethylamino)methylene)amino)phenyl ester<br>Dicarzol<br>Formetanat<br>Methanimidamide, N,N-dimethyl-N'-[3-[[(methylamino)carbonyl]oxy]phenyl]-<br>Methylcarbamic acid ester with N'-(m-hydroxyphenyl)-N,N-dimethylformamidine<br>Phenol, m-[[(dimethylamino)methylene]amino]-, methylcarbamate (ester)<br>m-[[(Dimethylamino)methylene]amino]phenyl methylcarbamate |
| **Inchi:** | InChI=1S/C11H15N3O2/c1-12-11(15)16-10-6-4-5-9(7-10)13-8-14(2)3/h4-8H,1-3H3,(H,12 |
| **InchiKey:** | RMFNNCGOSPBBAD-UHFFFAOYSA-N |
| **Formula:** | C11H15N3O2 |
| **SMILES:** | CNC(=O)Oc1cccc(N=CN(C)C)c1 |
| **Mol. weight [g/mol]:** | 221.26 |
| **CAS:** | 22259-30-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -86.89 | kJ/mol | Joback Method |
| hvap | 63.97 | kJ/mol | Joback Method |
| log10ws | -2.34 | | Aqueous Solubility Prediction Method |
| log10ws | -2.34 | | Estimated Solubility Method |
| logp | 1.626 | | Crippen Method |
| mcvol | 175.170 | ml/mol | McGowan Method |
| pc | 2485.07 | kPa | Joback Method |
| rinpol | 2117.00 | | NIST Webbook |
| rinpol | 2117.00 | | NIST Webbook |
| tb | 698.32 | K | Joback Method |
| tc | 919.34 | K | Joback Method |

# Sources

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|---|---|
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C22259309&Units=SI |
| **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 |

# Legend

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|---|---|
| **hf:** | Enthalpy of formation 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |