

N''-(4-ethoxy-phenyl)-N,N,N',N'-tetramethyl-guanidine

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|----------------------|--|
| Inchi: | InChI=1S/C13H21N3O/c1-6-17-12-9-7-11(8-10-12)14-13(15(2)3)16(4)5/h7-10H,6H2,1-5H |
| InchiKey: | HBZBTDXIKBUTFJ-UHFFFAOYSA-N |
| Formula: | C13H21N3O |
| SMILES: | CCOc1ccc(N=C(N(C)C)N(C)C)cc1 |
| Mol. weight [g/mol]: | 235.33 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -11.32 | kJ/mol | Joback Method |
| hvap | 57.36 | kJ/mol | Joback Method |
| log10ws | -1.96 | | Crippen Method |
| logp | 2.196 | | Crippen Method |
| mcvol | 201.780 | ml/mol | McGowan Method |
| pc | 1938.95 | kPa | Joback Method |
| rinpol | 1806.00 | | NIST Webbook |
| rinpol | 1806.00 | | NIST Webbook |
| tb | 652.36 | K | Joback Method |
| tc | 861.41 | K | 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=R153041&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-------|---|
| 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 |

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