

Butalamine

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| Other names: | 1,2-Ethanediamine, N,N-dibutyl-N'-(3-phenyl-1,2,4-oxadiazol-5-yl)-5-([2-(Dibutylamino)ethyl]amino)-3-phenyl-1,2,4-oxadiazole N,N-Dibutyl-N'-(3-phenyl-1,2,4-oxadiazol-5-yl)-1,2-ethanediamine |
| Inchi: | InChI=1S/C18H28N4O/c1-3-5-13-22(14-6-4-2)15-12-19-18-20-17(21-23-18)16-10-8-7-9- |
| InchiKey: | VYWQZAARVNRSTR-UHFFFAOYSA-N |
| Formula: | C18H28N4O |
| SMILES: | CCCCN(CCCC)CCNc1nc(-c2ccccc2)no1 |
| Mol. weight [g/mol]: | 316.44 |
| CAS: | 22131-35-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -9.69 | | Crippen Method |
| logp | 4.051 | | Crippen Method |
| mcvol | 267.050 | ml/mol | McGowan Method |
| rinpol | 2457.00 | | NIST Webbook |
| rinpol | 2450.00 | | NIST Webbook |
| rinpol | 2490.00 | | NIST Webbook |
| rinpol | 2450.00 | | NIST Webbook |
| rinpol | 2490.00 | | NIST Webbook |
| rinpol | 2457.00 | | NIST Webbook |
| rinpol | 2450.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemed.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C22131357&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpola: | Non-polar retention indices |

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