

Oxazole, 2,2'-(1,4-phenylene)bis[4-methyl-5-phenyl-

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| Other names: | Oxazole, 2,2'-p-phenylenebis[4-methyl-5-phenyl-Dimethyl-POPOP 1,4-Bis-2-(4-methyl-5-phenyloxazoyle)benzene 2,2'-p-Phenylenebis(4-methyl-5-phenyl)oxazole 1,4-di-(2-(4-Methyl-5-phenyloxazole))-benzene 1,4-Bis(4-methyl-5-phenyloxazole-2-yl)benzene 4-Methyl-2-[4-(4-methyl-5-phenyl-1,3-oxazole-2-yl)phenyl]-5-phenyl-1,3-oxazole 2,2'-(1,4-Phenylene)bis(4-methyl-5-phenyl)oxazole |
| Inchi: | InChI=1S/C26H20N2O2/c1-17-23(19-9-5-3-6-10-19)29-25(27-17)21-13-15-22(16-14-21) |
| InchiKey: | VLDFXDUAENINOO-UHFFFAOYSA-N |
| Formula: | C26H20N2O2 |
| SMILES: | <chem>Cc1nc(-c2ccc(-c3nc(C)c(-c4ccccc4)o3)cc2)oc1-c1ccccc1</chem> |
| Mol. weight [g/mol]: | 392.45 |
| CAS: | 3073-87-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -19.83 | | Crippen Method |
| logp | 6.947 | | Crippen Method |
| mcpvol | 298.700 | ml/mol | McGowan Method |
| rinpol | 3618.00 | | NIST Webbook |
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| rinpol | 3618.00 | | NIST Webbook |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|--------|-----------------|--------------|
| hsubt | 150.00 | kJ/mol | 480.00 | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3073878&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|--|
| hsubt: | Enthalpy of sublimation at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpol: | Non-polar retention indices |

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