

1,3,5-Triazine-2,4-diamine, 6-phenyl-

| | |
|-----------------------------|---|
| Other names: | s-Triazine, 2,4-diamino-6-phenyl- Benzoguanamine Benzoguanimine ENT 60118 2,4-Diamino-6-phenyl-s-triazine 2,4-Diamino-6-phenyl-1,3,5-triazine 2,6-Diamino-4-phenyl-1,3,5-triazine 6-Phenyl-1,3,5-triazine-2,4-diamine USAF RH-5 2-Phenyl-4,6-diamino-s-triazine 2-Phenyl-4,6-diamino-1,3,5-triazine 4,6-Diamino-2-phenyl-s-triazine NSC 3267 6-phenyl-1,3,5-triazine-2,4-diyldiamine |
| Inchi: | InChI=1S/C9H9N5/c10-8-12-7(13-9(11)14-8)6-4-2-1-3-5-6/h1-5H,(H4,10,11,12,13,14) |
| InchiKey: | GZVHEAJQGPRDLQ-UHFFFAOYSA-N |
| Formula: | C9H9N5 |
| SMILES: | <chem>Nc1nc(N)nc(-c2ccccc2)n1</chem> |
| Mol. weight [g/mol]: | 187.20 |
| CAS: | 91-76-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.64 | | Crippen Method |
| logp | 0.703 | | Crippen Method |
| mvol | 140.050 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C91769&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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

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