

Bis-(o-aminophenyl)-2,2'-dibenzimidazole oxide

Inchi: InChI=1S/C26H20N6O/c27-19-7-3-1-5-17(19)25-29-21-11-9-15(13-23(21)31-25)33-16-10
InchiKey: FZSYQUANOMQFJO-UHFFFAOYSA-N
Formula: C26H20N6O
SMILES: Nc1cccc1-c1nc2ccc(Oc3ccc4nc(-c5ccccc5N)[nH]c4c3)cc2[nH]1
Mol. weight [g/mol]: 432.48
CAS: 25829-64-5

Physical Properties

| Property code | Value | Unit | Source |
|---------------|------------------|--------|----------------|
| chs | -13191.00 ± 6.00 | kJ/mol | NIST Webbook |
| hfs | 102.00 ± 10.00 | kJ/mol | NIST Webbook |
| log10ws | -9.16 | | Crippen Method |
| logp | 4.766 | | Crippen Method |
| mcvol | 317.590 | ml/mol | McGowan Method |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C25829645&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

chs: Standard solid enthalpy of combustion
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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