

Tetrazobenzene-beta-naphthol

Inchi: InChI=1S/C22H16N4O/c27-22-20-9-5-4-6-16(20)10-15-21(22)26-25-19-13-11-18(12-14-
InchiKey: CWZMDLJDHVNFPS-QSZPNPOGSA-N
Formula: C22H16N4O
SMILES: Oc1c(N=Nc2ccc(N=Nc3ccccc3)cc2)ccc2ccccc12
Mol. weight [g/mol]: 352.39

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 297.44 | kJ/mol | Joback Method |
| hvap | 100.71 | kJ/mol | Joback Method |
| log10ws | -6.91 | | Crippen Method |
| logp | 7.376 | | Crippen Method |
| mcvol | 267.290 | ml/mol | McGowan Method |
| pc | 1603.85 | kPa | Joback Method |
| tb | 1190.76 | K | Joback Method |
| tc | 1490.29 | K | Joback Method |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003841&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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>

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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