

# 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

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**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](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## 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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