

Benzenamine, N-[(4-methoxyphenyl)methylidene]-3-nitro-

Other names: p-methoxybenzylidene-(3-nitrophenyl)-amine
Inchi: InChI=1S/C14H12N2O3/c1-19-14-7-5-11(6-8-14)10-15-12-3-2-4-13(9-12)16(17)18/h2-10
InchiKey: CXQR CMDXOBUAQA-UHFFFAOYSA-N
Formula: C14H12N2O3
SMILES: COc1ccc(C=Nc2cccc([N+](=O)[O-])c2)cc1
Mol. weight [g/mol]: 256.26

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 57.07 | kJ/mol | Joback Method |
| hvap | 74.95 | kJ/mol | Joback Method |
| log10ws | -4.11 | | Crippen Method |
| logp | 3.354 | | Crippen Method |
| mcvol | 189.570 | ml/mol | McGowan Method |
| pc | 2402.92 | kPa | Joback Method |
| rinpol | 2506.00 | | NIST Webbook |
| rinpol | 2506.00 | | NIST Webbook |
| tb | 833.98 | K | Joback Method |
| tc | 1103.23 | K | Joback Method |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U350566&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation at standard conditions

| | |
|---------------------------------------|---|
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀w_s: | Log ₁₀ of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mc_{vol}: | McGowan's characteristic volume |
| p_c: | Critical Pressure |
| r_{inpol}: | Non-polar retention indices |
| t_b: | Normal Boiling Point Temperature |
| t_c: | Critical Temperature |

Latest version available from:

<https://www.cheméo.com/cid/116-386-5/Benzenamine-N-4-methoxyphenyl-methylidene-3-nitro.pdf>

Generated by Cheméo on 2024-04-26 19:00:17.50060648 +0000 UTC m=+16447266.421183799.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.