

# P-phenylazo carbanilic acid, n-hexyl ester

|                             |                                                                                 |
|-----------------------------|---------------------------------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C19H23N3O2/c1-2-3-4-8-15-24-19(23)20-16-11-13-18(14-12-16)22-21-17-9-6 |
| <b>InchiKey:</b>            | RHHHUVCMNUYPHB-QURGRASLSA-N                                                     |
| <b>Formula:</b>             | C19H23N3O2                                                                      |
| <b>SMILES:</b>              | CCCCCOC(=O)Nc1ccc(N=Nc2ccccc2)cc1                                               |
| <b>Mol. weight [g/mol]:</b> | 325.40                                                                          |
| <b>CAS:</b>                 | 94915-64-7                                                                      |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -118.01 | kJ/mol | Joback Method  |
| hvap          | 85.36   | kJ/mol | Joback Method  |
| log10ws       | -5.87   |        | Crippen Method |
| logp          | 6.231   |        | Crippen Method |
| mcvol         | 264.130 | ml/mol | McGowan Method |
| pc            | 1481.57 | kPa    | Joback Method  |
| tb            | 968.12  | K      | Joback Method  |
| tc            | 1207.21 | K      | Joback Method  |

## Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C94915647&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C94915647&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |

|               |                                     |
|---------------|-------------------------------------|
| <b>logp:</b>  | Octanol/Water partition coefficient |
| <b>mcvol:</b> | McGowan's characteristic volume     |
| <b>pc:</b>    | Critical Pressure                   |
| <b>tb:</b>    | Normal Boiling Point Temperature    |
| <b>tc:</b>    | Critical Temperature                |

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