

Phenol, 4-nitroso-

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| Other names: | Phenol, p-nitroso- p-Nitrosophenol Nitrosophenol 4-Nitrosophenol Quinone monoxime p-Chinonmonoxim 4-Nitrosofenol Benzoquinone monooxime NSC 3124 |
| Inchi: | InChI=1S/C6H5NO2/c8-6-3-1-5(7-9)2-4-6/h1-4,8H |
| InchiKey: | JSTCPNFKICNNO-UHFFFAOYSA-N |
| Formula: | C6H5NO2 |
| SMILES: | O=Nc1ccc(O)cc1 |
| Mol. weight [g/mol]: | 123.11 |
| CAS: | 104-91-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -276.14 | kJ/mol | Joback Method |
| hvap | 53.34 | kJ/mol | Joback Method |
| log10ws | -1.78 | | Crippen Method |
| logp | 1.790 | | Crippen Method |
| mcvol | 89.060 | ml/mol | McGowan Method |
| pc | 5636.27 | kPa | Joback Method |
| tb | 507.38 | K | Joback Method |
| tc | 736.25 | K | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C104916&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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 |
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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<https://www.chemeo.com/cid/69-978-1/Phenol-4-nitroso.pdf>

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