

P-phenylenediamine, n,n'-bis(p-biphenyl)-

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| Inchi: | InChI=1S/C30H24N2/c1-3-7-23(8-4-1)25-11-15-27(16-12-25)31-29-19-21-30(22-20-29)3 |
| InchiKey: | ZBZGMYOKPNRAIU-UHFFFAOYSA-N |
| Formula: | C30H24N2 |
| SMILES: | c1ccc(-c2ccc(Nc3ccc(Nc4ccc(-c5ccccc5)cc4)cc3)cc2)cc1 |
| Mol. weight [g/mol]: | 412.52 |
| CAS: | 128049-24-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 913.66 | kJ/mol | Joback Method |
| hf | 592.65 | kJ/mol | Joback Method |
| hfus | 52.69 | kJ/mol | Joback Method |
| hvap | 108.61 | kJ/mol | Joback Method |
| log10ws | -10.29 | | Crippen Method |
| logp | 8.508 | | Crippen Method |
| mcvol | 334.720 | ml/mol | McGowan Method |
| pc | 1649.77 | kPa | Joback Method |
| tb | 1134.48 | K | Joback Method |
| tc | 1417.67 | K | Joback Method |
| tf | 702.84 | K | Joback Method |
| vc | 1.246 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1082.80 | J/molxK | 1134.48 | Joback Method |
| cpg | 1095.84 | J/molxK | 1181.68 | Joback Method |
| cpg | 1108.10 | J/molxK | 1228.88 | Joback Method |
| cpg | 1119.86 | J/molxK | 1276.08 | Joback Method |
| cpg | 1131.39 | J/molxK | 1323.27 | Joback Method |
| cpg | 1142.93 | J/molxK | 1370.47 | Joback Method |
| cpg | 1154.76 | J/molxK | 1417.67 | Joback Method |

Sources

| | |
|------------------------|---|
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C128049241&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion 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 |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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