# Phenol, 4-[2-(methylamino)ethyl]-

| | |
|---|---|
| **Other names:** | Phenol, p-[2-(methylamino)ethyl]- |
| | N-Methyltyramine |
| | 4-Hydroxy-N-methylphenethylamine |
| | p-(2-(Methylamino)ethyl)phenol |
| | Tyramine, N-methyl- |
| | WIN 5582 |
| | N-Methyl-p-tyramine |
| | 4-[2-(Methylamino)ethyl]phenol |
| | NSC 113958 |
| **Inchi:** | InChI=1S/C9H13NO/c1-10-7-6-8-2-4-9(11)5-3-8/h2-5,10-11H,6-7H2,1H3 |
| **InchiKey:** | AXVZFRBSCNEKPQ-UHFFFAOYSA-N |
| **Formula:** | C9H13NO |
| **SMILES:** | CNCCc1ccc(O)cc1 |
| **Mol. weight [g/mol]:** | 151.21 |
| **CAS:** | 370-98-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 72.08 | kJ/mol | Joback Method |
| hf | -116.40 | kJ/mol | Joback Method |
| hfus | 23.99 | kJ/mol | Joback Method |
| hvap | 57.35 | kJ/mol | Joback Method |
| log10ws | -1.43 | | Crippen Method |
| logp | 1.154 | | Crippen Method |
| mcvol | 129.760 | ml/mol | McGowan Method |
| pc | 3960.52 | kPa | Joback Method |
| tb | 562.79 | K | Joback Method |
| tc | 784.77 | K | Joback Method |
| tf | 381.99 | K | Joback Method |
| vc | 0.432 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| cpg | 312.73 | J/mol×K | 562.79 | Joback Method |
| cpg | 325.57 | J/mol×K | 599.79 | Joback Method |
| cpg | 337.52 | J/mol×K | 636.78 | Joback Method |
| cpg | 348.66 | J/mol×K | 673.78 | Joback Method |
| cpg | 359.07 | J/mol×K | 710.78 | Joback Method |
| cpg | 368.84 | J/mol×K | 747.77 | Joback Method |
| cpg | 378.03 | J/mol×K | 784.77 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C370989&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

**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