# Aniline mustard

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|---|---|
| **Other names:** | Benzenamine, N,N-bis(2-chloroethyl)- |
| | Aniline, N,N-bis(2-chloroethyl)- |
| | N,N-Bis(2-chloroethyl)aniline |
| | «beta»,«beta»'-Dichlorodiethylaniline |
| | N,N-Di(2-chloroethyl)aniline |
| | Lymphochin |
| | Lymphocin |
| | Lymphoquin |
| | NCS-18429 |
| | A 14489 |
| | CB 1074 |
| | Lymphchin |
| | Lymphoquine |
| | Mesylerythrol |
| | NSC-18429 |
| | SK 592 |
| | TL 476 |
| | Anilinlost |
| | N,N-Bis(2-chloroethyl)benzenamine |
| **Inchi:** | InChI=1S/C10H13Cl2N/c11-6-8-13(9-7-12)10-4-2-1-3-5-10/h1-5H,6-9H2 |
| **InchiKey:** | ROSJKFFLIXTTAW-UHFFFAOYSA-N |
| **Formula:** | C10H13Cl2N |
| **SMILES:** | ClCCN(CCCl)c1ccccc1 |
| **Mol. weight [g/mol]:** | 218.12 |
| **CAS:** | 553-27-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 232.65 | kJ/mol | Joback Method |
| hf | 22.85 | kJ/mol | Joback Method |
| hfus | 27.11 | kJ/mol | Joback Method |
| hvap | 50.94 | kJ/mol | Joback Method |
| log10ws | -2.52 | | Crippen Method |
| logp | 2.971 | | Crippen Method |
| mcvol | 162.460 | ml/mol | McGowan Method |
| pc | 2704.22 | kPa | Joback Method |
| tb | 542.18 | K | Joback Method |

| | | | |
|---|---|---|---|
| tc | 754.71 | K | Joback Method |
| tf | 319.00 ± 1.00 | K | NIST Webbook |
| vc | 0.604 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 346.78 | J/mol×K | 542.18 | Joback Method |
| cpg | 360.97 | J/mol×K | 577.60 | Joback Method |
| cpg | 374.22 | J/mol×K | 613.02 | Joback Method |
| cpg | 386.56 | J/mol×K | 648.44 | Joback Method |
| cpg | 398.06 | J/mol×K | 683.86 | Joback Method |
| cpg | 408.77 | J/mol×K | 719.29 | Joback Method |
| cpg | 418.72 | J/mol×K | 754.71 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 442.00 ± 1.00 | K | 2.10 | NIST Webbook |
| tbrp | 437.00 | K | 1.90 | NIST Webbook |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C553275&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |