# hexestrol bis(«beta»-diethyl-aminoethyl ether)

**Inchi:** InChI=1S/C32H52N2O2/c1-7-13-31(27-15-19-29(20-16-27)35-25-23-33(9-3)10-4)32(14-8
**InchiKey:** GKMRDSMWVSUEQQ-UHFFFAOYSA-N
**Formula:** C32H52N2O2
**SMILES:** CCCC(c1ccc(OCCN(CC)CC)cc1)C(CCC)c1ccc(OCCN(CC)CC)cc1
**Mol. weight [g/mol]:** 496.77

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 430.80 | kJ/mol | Joback Method |
| hf | -393.63 | kJ/mol | Joback Method |
| hfus | 67.31 | kJ/mol | Joback Method |
| hvap | 100.83 | kJ/mol | Joback Method |
| log10ws | -7.89 | | Crippen Method |
| logp | 7.595 | | Crippen Method |
| mcvol | 445.920 | ml/mol | McGowan Method |
| pc | 738.42 | kPa | Joback Method |
| rinpol | 3205.00 | | NIST Webbook |
| rinpol | 3255.00 | | NIST Webbook |
| rinpol | 3205.00 | | NIST Webbook |
| tb | 1063.72 | K | Joback Method |
| tc | 1306.60 | K | Joback Method |
| tf | 607.68 | K | Joback Method |
| vc | 1.671 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1576.63 | J/mol×K | 1063.72 | Joback Method |
| cpg | 1596.61 | J/mol×K | 1104.20 | Joback Method |
| cpg | 1614.81 | J/mol×K | 1144.68 | Joback Method |
| cpg | 1631.35 | J/mol×K | 1185.16 | Joback Method |
| cpg | 1646.37 | J/mol×K | 1225.64 | Joback Method |
| cpg | 1660.00 | J/mol×K | 1266.12 | Joback Method |
| cpg | 1672.38 | J/mol×K | 1306.60 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R211088&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 |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |