# Dexoxadrol

**Inchi:** InChI=1S/C20H23NO2/c1-3-9-16(10-4-1)20(17-11-5-2-6-12-17)22-15-19(23-20)18-13-7-8
**InchiKey:** HGKAMARNFGKMLC-UHFFFAOYSA-N
**Formula:** C20H23NO2
**SMILES:** c1ccc(C2(c3ccccc3)OCC(C3CCCCN3)O2)cc1
**Mol. weight [g/mol]:** 309.40
**CAS:** 631-06-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 305.61 | kJ/mol | Joback Method |
| hf | -99.56 | kJ/mol | Joback Method |
| hfus | 41.73 | kJ/mol | Joback Method |
| hvap | 79.67 | kJ/mol | Joback Method |
| log10ws | -4.54 | | Crippen Method |
| logp | 3.445 | | Crippen Method |
| mcvol | 245.140 | ml/mol | McGowan Method |
| pc | 2329.27 | kPa | Joback Method |
| rinpol | 2340.00 | | NIST Webbook |
| rinpol | 2340.00 | | NIST Webbook |
| rinpol | 2340.00 | | NIST Webbook |
| tb | 843.21 | K | Joback Method |
| tc | 1126.02 | K | Joback Method |
| tf | 564.11 | K | Joback Method |
| vc | 0.889 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 793.95 | J/mol×K | 843.21 | Joback Method |
| cpg | 817.02 | J/mol×K | 890.34 | Joback Method |
| cpg | 838.91 | J/mol×K | 937.48 | Joback Method |
| cpg | 859.97 | J/mol×K | 984.61 | Joback Method |
| cpg | 880.54 | J/mol×K | 1031.75 | Joback Method |
| cpg | 900.97 | J/mol×K | 1078.88 | Joback Method |

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|---|---|---|---|---|
| cpg | 921.59 | J/mol×K | 1126.02 | 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=C631061&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 |