# 5-(((1R,3aR,4S,6aR)-4-(Benzo[d][1,3]dioxol-5-yl)he

**Inchi:** InChI=1S/C20H18O7/c1-3-15-17(25-9-23-15)5-11(1)19-13-7-22-20(14(13)8-21-19)27-12
**InchiKey:** ZZMNWJVJUKMZJY-UHFFFAOYSA-N
**Formula:** C20H18O7
**SMILES:** c1cc2c(cc1OC1OCC3C(c4ccc5c(c4)OCO5)OCC13)OCO2
**Mol. weight [g/mol]:** 370.35
**CAS:** 526-07-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -99.10 | kJ/mol | Joback Method |
| hf | -674.29 | kJ/mol | Joback Method |
| hfus | 71.48 | kJ/mol | Joback Method |
| hvap | 96.78 | kJ/mol | Joback Method |
| log10ws | -4.27 | | Crippen Method |
| logp | 2.883 | | Crippen Method |
| mcvol | 242.790 | ml/mol | McGowan Method |
| pc | 2410.00 | kPa | Joback Method |
| rinpol | 3208.40 | | NIST Webbook |
| rinpol | 3208.40 | | NIST Webbook |
| tb | 949.90 | K | Joback Method |
| tc | 1212.72 | K | Joback Method |
| tf | 664.45 | K | Joback Method |
| vc | 0.895 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 842.77 | J/mol×K | 949.90 | Joback Method |
| cpg | 911.82 | J/mol×K | 1168.92 | Joback Method |
| cpg | 898.98 | J/mol×K | 1125.11 | Joback Method |
| cpg | 885.86 | J/mol×K | 1081.31 | Joback Method |
| cpg | 872.26 | J/mol×K | 1037.51 | Joback Method |
| cpg | 857.96 | J/mol×K | 993.70 | Joback Method |
| cpg | 924.58 | J/mol×K | 1212.72 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0018052 | Pa×s | 949.90 | Joback Method |
| dvisc | 0.0020062 | Pa×s | 902.32 | Joback Method |
| dvisc | 0.0022560 | Pa×s | 854.75 | Joback Method |
| dvisc | 0.0025722 | Pa×s | 807.17 | Joback Method |
| dvisc | 0.0029813 | Pa×s | 759.60 | Joback Method |
| dvisc | 0.0035242 | Pa×s | 712.02 | Joback Method |
| dvisc | 0.0042671 | Pa×s | 664.45 | Joback Method |

# Sources

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|---|---|
| **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=C526078&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 |
| **dvisc:** | Dynamic viscosity |
| **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 |