# 2-(3',4'-Methylenedioxy)phenyl-4-keto-1,3-benzoth

**Inchi:** InChI=1S/C15H10O4S/c16-14-10-3-1-2-4-13(10)20-15(19-14)9-5-6-11-12(7-9)18-8-17-1
**InchiKey:** FFXRKNMJMJPRBJ-UHFFFAOYSA-N
**Formula:** C15H10O4S
**SMILES:** O=C1OC(c2ccc3c(c2)OCO3)Sc2ccccc21
**Mol. weight [g/mol]:** 286.30
**CAS:** 97192-88-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 47.37 | kJ/mol | Joback Method |
| hf | -242.94 | kJ/mol | Joback Method |
| hfus | 41.72 | kJ/mol | Joback Method |
| hvap | 79.42 | kJ/mol | Joback Method |
| log10ws | -4.71 | | Crippen Method |
| logp | 3.377 | | Crippen Method |
| mcvol | 188.500 | ml/mol | McGowan Method |
| pc | 3376.28 | kPa | Joback Method |
| tb | 829.82 | K | Joback Method |
| tc | 1116.87 | K | Joback Method |
| tf | 617.19 | K | Joback Method |
| vc | 0.682 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 543.41 | J/mol×K | 829.82 | Joback Method |
| cpg | 556.84 | J/mol×K | 877.66 | Joback Method |
| cpg | 568.98 | J/mol×K | 925.50 | Joback Method |
| cpg | 579.97 | J/mol×K | 973.35 | Joback Method |
| cpg | 589.94 | J/mol×K | 1021.19 | Joback Method |
| cpg | 599.03 | J/mol×K | 1069.03 | Joback Method |
| cpg | 607.38 | J/mol×K | 1116.87 | Joback Method |

# Sources

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|---|---|
| **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=C97192886&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |