# Tiapride

**Inchi:** InChI=1S/C15H24N2O4S/c1-5-17(6-2)10-9-16-15(18)13-11-12(22(4,19)20)7-8-14(13)21-
**InchiKey:** JTVPZMFULRWINT-UHFFFAOYSA-N
**Formula:** C15H24N2O4S
**SMILES:** CCN(CC)CCNC(=O)c1cc(S(C)(=O)=O)ccc1OC
**Mol. weight [g/mol]:** 328.43
**CAS:** 51012-32-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -333.72 | kJ/mol | Joback Method |
| hf | -716.49 | kJ/mol | Joback Method |
| hfus | 50.15 | kJ/mol | Joback Method |
| hvap | 88.85 | kJ/mol | Joback Method |
| log10ws | -2.29 | | Crippen Method |
| logp | 1.170 | | Crippen Method |
| mcvol | 253.940 | ml/mol | McGowan Method |
| pc | 2173.43 | kPa | Joback Method |
| rinpol | 2850.00 | | NIST Webbook |
| rinpol | 2850.00 | | NIST Webbook |
| tb | 765.92 | K | Joback Method |
| tc | 961.20 | K | Joback Method |
| tf | 506.12 | K | Joback Method |
| vc | 0.971 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 734.43 | J/mol×K | 765.92 | Joback Method |
| cpg | 749.59 | J/mol×K | 798.47 | Joback Method |
| cpg | 763.68 | J/mol×K | 831.01 | Joback Method |
| cpg | 776.72 | J/mol×K | 863.56 | Joback Method |
| cpg | 788.72 | J/mol×K | 896.10 | Joback Method |
| cpg | 799.70 | J/mol×K | 928.65 | Joback Method |
| cpg | 809.67 | J/mol×K | 961.20 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C51012329&Units=SI |

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