# N-(2-Hydroxy-propionyl)-4-methyl-benzenesulfona O-pentafluoropropionyl-

**Inchi:** InChI=1S/C13H12F5NO5S/c1-7-3-5-9(6-4-7)25(22,23)19-10(20)8(2)24-11(21)12(14,15)1

**Inchikey:** UOMFZVOEHCLLGM-UHFFFAOYSA-N

**Formula:** C13H12F5NO5S

**SMILES:** Cc1ccc(S(=O)(=O)NC(=O)C(C)OC(=O)C(F)(F)C(F)(F)F)cc1

**Mol. weight [g/mol]:** 389.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1551.44 | kJ/mol | Joback Method |
| hf | -1847.18 | kJ/mol | Joback Method |
| hfus | 40.99 | kJ/mol | Joback Method |
| hvap | 81.38 | kJ/mol | Joback Method |
| log10ws | -3.64 | | Crippen Method |
| logp | 1.929 | | Crippen Method |
| mcvol | 226.200 | ml/mol | McGowan Method |
| pc | 2374.90 | kPa | Joback Method |
| rinpol | 1824.00 | | NIST Webbook |
| rinpol | 1824.00 | | NIST Webbook |
| tb | 746.06 | K | Joback Method |
| tc | 937.45 | K | Joback Method |
| tf | 481.31 | K | Joback Method |
| vc | 0.908 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 645.42 | J/mol×K | 746.06 | Joback Method |
| cpg | 656.58 | J/mol×K | 777.96 | Joback Method |
| cpg | 666.79 | J/mol×K | 809.86 | Joback Method |
| cpg | 676.09 | J/mol×K | 841.76 | Joback Method |
| cpg | 684.50 | J/mol×K | 873.65 | Joback Method |
| cpg | 692.08 | J/mol×K | 905.55 | Joback Method |
| cpg | 698.85 | J/mol×K | 937.45 | Joback Method |

# Sources

| | |
|---|---|
| **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=U374248&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |