# Quinethazone

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|---|---|
| **Other names:** | 2-Ethyl-7-chloro-1,2,3,4-tetrahydro-4-oxoquinazoline-6-sulfonamide |
| | 6-Quinazolinesulfonamide, 7-chloro-2-ethyl-1,2,3,4-tetrahydro-4-oxo- |
| | 7-Chloro-2-ethyl-1,2,3,4-tetrahydro-4-oxo-6-quinazolinesulfonamide |
| | 7-Chloro-2-ethyl-1,2,3,4-tetrahydro-4-oxo-6-quinzaolinesulfonamide |
| | 7-Chloro-2-ethyl-1,2,3,4-tetrahydro-4-oxo-6-sulfamoylquinazoline |
| | 7-Chloro-2-ethyl-6-sulfamoyl-1,2,3,4-tetrahydro-4-quinazolinone |
| | 7-chloro-2-ethyl-4-oxo-2,3-dihydro-1H-quinazoline-6-sulfonamide |
| | Aquamox |
| | CL 36010 |
| | Chinetazone |
| | Hydromox |
| | Idrokin |
| | Quinethazon |
| | Quinethazone Me |
| | Quinethazonum |
| **Inchi:** | InChI=1S/C10H12ClN3O3S/c1-2-9-13-7-4-6(11)8(18(12,16)17)3-5(7)10(15)14-9/h3-4,9,1 |
| **InchiKey:** | AGMMTXLNIQSRCG-UHFFFAOYSA-N |
| **Formula:** | C10H12ClN3O3S |
| **SMILES:** | CCC1NC(=O)c2cc(S(N)(=O)=O)c(Cl)cc2N1 |
| **Mol. weight [g/mol]:** | 289.74 |
| **CAS:** | 73-49-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -195.70 | kJ/mol | Joback Method |
| hf | -478.35 | kJ/mol | Joback Method |
| hfus | 50.03 | kJ/mol | Joback Method |
| hvap | 93.62 | kJ/mol | Joback Method |
| log10ws | -3.29 | | Aqueous Solubility Prediction Method |
| log10ws | -3.29 | | Estimated Solubility Method |
| logp | 0.879 | | Crippen Method |
| mcvol | 188.980 | ml/mol | McGowan Method |
| pc | 4583.94 | kPa | Joback Method |
| rinpol | 3000.00 | | NIST Webbook |
| rinpol | 3000.00 | | NIST Webbook |

| | | | |
|---|---|---|---|
| tb | 803.49 | K | Joback Method |
| tc | 1054.38 | K | Joback Method |
| tf | 710.88 | K | Joback Method |
| vc | 0.722 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 518.68 | J/mol×K | 803.49 | Joback Method |
| cpg | 530.98 | J/mol×K | 845.30 | Joback Method |
| cpg | 541.90 | J/mol×K | 887.12 | Joback Method |
| cpg | 551.40 | J/mol×K | 928.93 | Joback Method |
| cpg | 559.43 | J/mol×K | 970.75 | Joback Method |
| cpg | 565.95 | J/mol×K | 1012.56 | Joback Method |
| cpg | 570.93 | J/mol×K | 1054.38 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C73494&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
**Estimated Solubility Method:** http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

# 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 |