

risperidone

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| Other names: | 3-[2-[4-(6-fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl]-6,7,8,9-tetrahydro-2-methyl-4H- |
| Inchi: | InChI=1S/C23H27FN4O2/c1-15-18(23(29)28-10-3-2-4-21(28)25-15)9-13-27-11-7-16(8-1 |
| InchiKey: | RAPZEAPATHNIPO-UHFFFAOYSA-N |
| Formula: | C23H27FN4O2 |
| SMILES: | Cc1nc2n(c(=O)c1CCN1CCC(c3noc4cc(F)ccc34)CC1)CCCC2 |
| Mol. weight [g/mol]: | 410.49 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|--|
| hfus | 41.87 | kJ/mol | Risperidone Solid-state characterization and pharmaceutical compatibility using thermal and non-thermal techniques |
| hfus | 43.94 | kJ/mol | Thermodynamics of risperidone and solubility in pure organic solvents |
| log10ws | -10.67 | | Crippen Method |
| logp | 3.590 | | Crippen Method |
| mcvol | 303.960 | ml/mol | McGowan Method |
| tf | 442.38 | K | Thermodynamics of risperidone and solubility in pure organic solvents |
| tf | 443.67 | K | Risperidone Solid-state characterization and pharmaceutical compatibility using thermal and non-thermal techniques |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---|
| cpl | 856.00 | J/molxK | 453.00 | Thermodynamics of risperidone and solubility in pure organic solvents |

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|-----|--------|---------|--------|---|
| cpl | 854.00 | J/molxK | 449.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cpl | 850.00 | J/molxK | 445.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cpl | 845.00 | J/molxK | 440.00 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cpl | 842.00 | J/molxK | 434.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cpl | 839.00 | J/molxK | 430.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 578.00 | J/molxK | 355.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 509.00 | J/molxK | 304.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 516.00 | J/molxK | 310.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 523.00 | J/molxK | 314.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 530.00 | J/molxK | 320.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 537.00 | J/molxK | 324.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 544.00 | J/molxK | 330.10 | Thermodynamics of risperidone and solubility in pure organic solvents |

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|-----|--------|---------|--------|---|
| cps | 551.00 | J/molxK | 334.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 558.00 | J/molxK | 340.00 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 564.00 | J/molxK | 345.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 571.00 | J/molxK | 350.00 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 502.00 | J/molxK | 300.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 583.00 | J/molxK | 359.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 590.00 | J/molxK | 365.00 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 597.00 | J/molxK | 370.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 602.00 | J/molxK | 375.00 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 609.00 | J/molxK | 380.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 615.00 | J/molxK | 384.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 621.00 | J/molxK | 390.00 | Thermodynamics of risperidone and solubility in pure organic solvents |

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|-----|--------|---------|--------|---|
| cps | 627.00 | J/mol×K | 394.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 634.00 | J/mol×K | 400.00 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 641.00 | J/mol×K | 405.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 647.00 | J/mol×K | 409.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 495.00 | J/mol×K | 294.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 489.00 | J/mol×K | 290.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 483.00 | J/mol×K | 284.90 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 480.00 | J/mol×K | 280.10 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 476.00 | J/mol×K | 275.00 | Thermodynamics of risperidone and solubility in pure organic solvents |
| cps | 471.00 | J/mol×K | 270.10 | Thermodynamics of risperidone and solubility in pure organic solvents |

Sources

Risperidone Solid-state characterization and compatibility using thermal and non-thermal techniques:

<https://www.doi.org/10.1016/j.tca.2013.06.032>

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamics of risperidone and solubility in pure organic solvents: <https://www.doi.org/10.1016/j.fluid.2014.04.028>

Legend

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|-----------------|---|
| cpl: | Liquid phase heat capacity |
| cps: | Solid phase heat capacity |
| hfus: | Enthalpy of fusion at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| tf: | Normal melting (fusion) point |

Latest version available from:

<https://www.chemeo.com/cid/101-395-1/risperidone.pdf>

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