risperidone

Other names: 3-[2-[4-(6-fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl]-6,7,8,9-tetrahydro-2-methyl-4F

InChl=1S/C23H27FN4O2/c1-15-18(23(29)28-10-3-2-4-21(28)25-15)9-13-27-11-7-16(8-12)

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	43.94	kJ/mol	Thermodynamics of risperidone and solubility in pure organic solvents
hfus	41.87	kJ/mol	Risperidone Solid-state characterization and pharmaceuticalcompatibility using thermal and non-thermal techniques
log10ws	-10.67		Crippen Method
logp	3.590		Crippen Method
mcvol	303.960	ml/mol	McGowan Method
tf	442.38	К	Thermodynamics of risperidone and solubility in pure organic solvents
tf	443.67	К	Risperidone Solid-state characterization and pharmaceuticalcompatibility using thermal and non-thermal techniques

Temperature Dependent Properties

P	Property code	Value	Unit	Temperature [K]	Source
	cpl	856.00	J/mol×K	453.00	Thermodynamics of risperidone and solubility in pure organic solvents

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 cpl 839.00 J/molxK 355.10 Thermodynamics of risperidone and solubility in pure organic solvents cps 578.00 J/molxK 304.90 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 530.00 J/molxK 310.10 Thermodynamics of risperidone and solubility in pure organic solvents cps 537.00 J/molxK 320.10 Thermodynamics of risperidone and solubility in pure organic solvents cps 537.00 J/molxK 320.10 Thermodynamics of risperidone and solubility in pure organic solvents cps 537.00 J/molxK 320.10 Thermodynamics of risperidone and solubility in pure organic solvents cps 537.00 J/molxK 320.10 Thermodynamics of risperidone and solubility in pure organic solvents cps 537.00 J/molxK 320.10 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 cps 544.00 J/molxK 330.10 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	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

McGowan Method: 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

Legend

cpl: Liquid phase heat capacitycps: Solid phase heat capacity

hfus: Enthalpy of fusion at standard conditions

log10ws:Log10 of Water solubility in mol/llogp:Octanol/Water partition coefficientmcvol:McGowan's characteristic volumetf:Normal melting (fusion) point

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