Ampyrone

Other names:	1,2-dihydro-1,5-dimethyl-2-phenyl-4-amino-3H-pyrazol-3-one 1,5-Dimethyl-2-phenyl-4-aminopyrazoline 3-Pyrazolin-5-one, 4-amino-2,3-dimethyl-1-phenyl- 3H-Pyrazol-3-one, 4-amino-1,2-dihydro-1,5-dimethyl-2-phenyl- 4-AAP 4-Amino-1,5-dimethyl-2-phenyl-3-pyrazolone 4-Amino-1-phenyl-2,3-dimethyl-5-pyrazolone 4-Amino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one 4-Aminoantipyrene 4-Aminoantipyrine 4-Aminophenazone 4-Amminoantipirina Aminoantipyrene Aminoantipyrin Aminoantipyrine Aminoazophenazone Aminoazophene Aminophenazone Antipyrine, 4-amino- Metapirazone NSC 60242 Solnapyrin-A Solvapyrin-A
Inchi:	InChI=1S/C11H13N3O/c1-8-10(12)11(15)14(13(8)2)9-6-4-3-5-7-9/h3-7H,12H2,1-2H3
InchiKey:	RLFWWDJHLFCNIJ-UHFFFAOYSA-N
Formula:	C11H13N3O
SMILES:	Cc1c(N)c(=O)n(-c2ccccc2)n1C
Mol. weight [g/mol]:	203.24
CAS:	83-07-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.62		Aqueous Solubility Prediction Method
log10ws	-0.62		Estimated Solubility Method
logp	1.067		Crippen Method

mcvol	158.440	ml/mol	McGowan Method
rinpol	1957.00		NIST Webbook
rinpol	1950.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	294.60	J/mol×K	323.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C83078&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Measurements for the solid solubilities of antipyrine, 4-aminoantipyrine and 4-dimethylaminoantipyrine in supercritical carbon dioxide: https://www.doi.org/10.1016/j.fluid.2009.04.019

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

cps: Solid phase heat capacity

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices