Aminopyrine

Other names:

(Dimethylamino)phenazone
(dimethylamino)analgesine
(dimethylamino)antipyrine
,3-Dimethyl-4-dimethylamino-1-phenyl-3-pyrazolin-5-one
1,5-Dimethyl-2-phenyl-4-dimethylamino-3-pyrazolone
1,5-Dimethyl-4-dimethylamino-2-phenyl-3-pyrazolone
1-Phenyl-2,3-dimethyl-4-(dimethylamino)-5-pyrazolone
1-Phenyl-2,3-dimethyl-4-dimethylaminopyrazol-5-one
1-Phenyl-2,3-dimethyl-4-dimethylaminopyrazolone-5
2,3-Dimethyl-4-dimethylamino-1-phenyl-5-pyrazolone
3-Pyrazolin-5-one, 4-(dimethylamino)-2,3-dimethyl-1-phenyl-
3-keto-1,5-Dimethyl-4-dimethylamino-2-phenyl-2,3-dihydropyrazole
3H-Pyrazol-3-one, 4-(dimethylamino)-1,2-dihydro-1,5-dimethyl-2-phenyl-
4-(Dimethylamino)antipyrine
4-(Dimethylamino)phenazone
4-Dimethylamino-1-phenyl-2,3-dimethylpyrazolone
4-Dimethylamino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one
4-Dimethylamino-2,3-dimethyl-1-phenyl-5-pyrazolone
4-N,N-Dimethylaminoantipyrine
4-dimethylaminoantipyrine
4-dimethylaminophenazone
Amidazofen
Amidazophen
Amidazophene
Amidofebrin
Amidofen
Amidophen
Amidophenazone
Amidopyrazoline
Amidopyrin
Amidopyrine
Aminofenazone
Aminophenazon
Aminophenazone
Aminopyrin
Anafebrina
Antipyrine, 4-(dimethylamino)-
Brufaneuxol
Dereuma
Dimapyrin

Dimethylamino-analgesine
Dimethylaminoantipyrine
Dimethylaminoazophene
Dimethylaminophenazon
Dimethylaminophenyldimethylpyrazolin
Dimethylaminophenyldimethylpyrazolone
Dimethylaminophenyldimethylpyrazone
Dipirin
Dipyrin
Dipyrine
Eufibron
Febrinina
Febron
Hyparon
Itamidone
Mamallet-A
Netsusarin
Novamidon
Piramidon
Piramidone
Pirazon
Piridol
Piromidina
Polinalin
Pyradone
Pyramidon
Pyramidone

Inchi: InChI=1S/C13H17N3O/c1-10-12(14(2)3)13(17)16(15(10)4)11-8-6-5-7-9-11/h5-9H,1-4H3
InchiKey: RMMXTBMQSGEXHJ-UHFFFAOYSA-N
Formula: C13H17N3O
SMILES: Cc1c(N(C)C)c(=O)n(-c2ccccc2)n1C
Mol. weight [g/mol]: 231.29
CAS: 58-15-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.73		Aqueous Solubility Prediction Method
log10ws	-0.36		Estimated Solubility Method

log10ws	-0.62		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.550		Crippen Method
mcvol	186.620	ml/mol	McGowan Method
rinpol	1940.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1903.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1935.00		NIST Webbook
rinpol	1877.00		NIST Webbook
rinpol	1879.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1903.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1903.00		NIST Webbook
tf	389.77	K	Aqueous Solubility Prediction Method

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58151&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

Legend

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point