Antipyrine

Other names:
1,2-Dihydro-1,5-dimethyl-2-phenyl-3H-pyrazol-3-one
1,5-Dimethyl-2-phenyl-3-pyrazolone
1-Phenyl-2,3-dimethyl-5-pyrazolone
1-Phenyl-2,3-dimethylpyrazole-5-one
2,3-Dimethyl-1-phenyl-3-pyrazolin-5-one
2,3-Dimethyl-1-phenyl-5-pyrazolone
3-Antipyrine
3H-Pyrazol-3-one, 1,2-dihydro-1,5-dimethyl-2-phenyl-
Analgesin
Analgesine
Anodynin
Anodynine
Antipirin
Antipyrene
Antipyrin
Antypirine
Apirelina
Azophen
Azophene
Dimethyloxychinizin
Dimethyloxyquinazine
Fenazon
Fenazone
Methozin
NSC 7945
Oxydimethylquinazine
Oxydimethylquinizine
Parodyne
Phenazon
Phenazone
Phenazone (pharmaceutical)
Phenazonum
Phenozone
Phenylon
Phenylone
Pyrazophyl
Sedatin
Sedatine

Inchi: InChI=1S/C11H12N2O/c1-9-8-11(14)13(12(9)2)10-6-4-3-5-7-10/h3-8H,1-2H3

InchiKey: VEQOALNAAJBPNY-UHFFFAOYSA-N

Formula: C11H12N2O
SMILES: Cc1cc(=O)n(-c2ccccc2)n1C
Mol. weight [g/mol]: 188.23
CAS: 60-80-0

Physical Properties

Property code	Value	Unit	Source
ie	7.86 ± 0.05	eV	NIST Webbook
ie	7.40	eV	NIST Webbook
log10ws	0.48		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	0.71		Estimated Solubility Method
logp	1.484		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
rinpol	1895.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1848.00		NIST Webbook
ripol	3082.00		NIST Webbook
tf	382.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	268.20	J/mol×K	323.00	NIST Webbook
hfust	24.52	kJ/mol	385.80	NIST Webbook

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=C60800&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
Measurement and correlation of solid-liquid equilibria for three binaries, ethanol-antipyrine, chloroform-antipyrine, and dimethyl ether-antipyrine:	https://www.doi.org/10.1016/j.fluid.2015.11.035

Legend

cps:	Solid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point