

Pyrazon

Other names:	1-Phenyl-4-amino-5-chloro-6-oxo-(1H)pyridazine 1-Phenyl-4-amino-5-chloropyridazin-6-one 1-Phenyl-4-amino-5-chloropyridaz-6-one 3(2H)-Pyridazinone, 5-amino-4-chloro-2-phenyl- 5-Amino-4-chloro-2,3-dihydro-3-oxo-2-phenylpyridazine 5-Amino-4-chloro-2-phenyl-3(2H)-pyridazinone 5-Amino-4-chloro-2-phenyl-3-pyridazinone 5-Amino-4-chloro-2-phenylpyridazin-3(2H)-one BAS 13033 Betoxon Burex Chloridazon Chloridazone Curbetan HS 119-1 PAC PCA PCA (pesticide) Phenazon Phenazone Phenazone (herbicide) Phenosane Pyramin Pyramine Suzon Tripart gladiator
Inchi:	InChI=1S/C10H8ClN3O/c11-9-8(12)6-13-14(10(9)15)7-4-2-1-3-5-7/h1-6H,12H2
InchiKey:	WYKYKTKDBLFHCY-UHFFFAOYSA-N
Formula:	C10H8ClN3O
SMILES:	<chem>Nc1cnn(-c2ccccc2)c(=O)c1Cl</chem>
Mol. weight [g/mol]:	221.64
CAS:	1698-60-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Estimated Solubility Method

logp	1.468		Crippen Method
mcvol	152.290	ml/mol	McGowan Method
tf	479.38 ± 0.20	K	NIST Webbook
tf	480.20 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	26.75	kJ/mol	479.20	NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1698608&Units=SI>

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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