Luminol

Other names:	1,4-Phthalazinedione, 5-amino-2,3-dihydro-
	1,2-Benzenedicarboxylic acid, 3-amino-, cyclic hydrazide
	3-Aminophthalhydrazide
	3-Aminophthalic acid hydrazide
	3-Aminophthalic hydrazide
	5-Amino-2,3-dihydro-1,4-phthalazinedione
	5-Amino-1,2,3,4-tetrahydro-1,4-phthalazinedione
	5-Amino-1,4-dihydroxyphthalazine
	5-Amino-2,3-dihydro-phthalazine-1,4-dione
	NSC 5064
	5-amino-1,2,3,4-tetrahydrophthalazine-1,4-dione
Inchi:	InChI=1S/C8H7N3O2/c9-5-3-1-2-4-6(5)8(13)11-10-7(4)12/h1-3H,9H2,(H,10,12)(H,11,13)
InchiKey:	HWYHZTIRURJOHG-UHFFFAOYSA-N
Formula:	C8H7N3O2
SMILES:	Nc1cccc2c(=O)[nH][nH]c(=O)c12
Mol. weight [g/mol]:	177.16
CAS:	521-31-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.19		Crippen Method
logp	-1.165		Crippen Method
mcvol	122.040	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C521313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume