

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
mccvol	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

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