

Acetic acid, (3,4-dihydro-5-nitro-4-oxo-6-pyrimidinyl)hydrazide

Inchi: InChI=1S/C6H7N5O4/c1-3(12)9-10-5-4(11(14)15)6(13)8-2-7-5/h2H,1H3,(H,9,12)(H2,7,8,
InchiKey: XSDRAAXSBITUQL-UHFFFAOYSA-N
Formula: C6H7N5O4
SMILES: CC(=O)NNc1nc[nH]c(=O)c1[N+](=O)[O-]
Mol. weight [g/mol]: 213.15
CAS: 30958-43-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.91		Crippen Method
logp	-1.341		Crippen Method
mcvol	136.420	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C30958431&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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