

Hexanal, 4-oxo-6-methylpyrimidin-2-ylhydrazone (keto form)

InChI: InChI=1S/C11H18N4O/c1-3-4-5-6-7-12-15-11-13-9(2)8-10(16)14-11/h7-8H,3-6H2,1-2H3
InChIKey: XQJXFRREHXVMNQ-KPKJPENVSA-N
Formula: C11H18N4O
SMILES: CCCCCC=NNc1nc(C)cc(=O)[nH]1
Mol. weight [g/mol]: 222.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.574		Crippen Method
mcvol	183.580	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009995&Units=SI>

Legend

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

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