

Ketone, 1,3-dimethyl-4-nitro-pyrazol-5-yl phenyl

InChI: InChI=1S/C12H11N3O3/c1-8-10(15(17)18)11(14(2)13-8)12(16)9-6-4-3-5-7-9/h3-7H,1-2H3

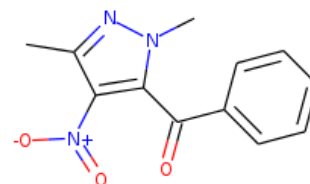
InChI Key: MDIJUXNXKCMMJW-UHFFFAOYSA-N

Formula: C12H11N3O3

SMILES: Cc1nn(C)c(C(=O)c2ccccc2)c1[N+](=O)[O-]

Molecular Weight: 245.23

CAS: 26308-46-3



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	1.87		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H11N3O3/c1-8-10\(15\(17\)18\)11\(14\(2\)13-8\)12\(16\)9-6-4-3-5-7-9/h3-7H,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H11N3O3/c1-8-10(15(17)18)11(14(2)13-8)12(16)9-6-4-3-5-7-9/h3-7H,1-2H3)

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

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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