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,1-2H

InchiKey: MDIJUXNXKCMMJW-UHFFFAOYSA-N

Formula: C12H11N3O3

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

Mol. weight [g/mol]: 245.23

CAS: 26308-46-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.61		Crippen Method
logp	1.868		Crippen Method
mcvol	175.670	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26308463&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume