3-Hydroxy-5-benzoyl-1,2,4-oxadiazole

Inchi: InChI=1S/C9H6N2O3/c12-7(6-4-2-1-3-5-6)8-10-9(13)11-14-8/h1-5H,(H,11,13)
InchiKey: VWNHDZBGJCWIPM-UHFFFAOYSA-N
Formula: C9H6N2O3
SMILES: O=C(c1ccccc1)c1nc(O)no1
Mol. weight [g/mol]: 190.16
CAS: 42837-65-0

Physical Properties

Property code	Value	Unit	Source
chs	-4356.40 ± 8.40	kJ/mol	NIST Webbook
log10ws	-6.24		Crippen Method
logp	1.006		Crippen Method
mcvol	127.720	ml/mol	McGowan Method

Sources

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=C42837650&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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