3-Benzoyl-5-hydroxy-1,2,4-oxadiazole

Inchi: InChI=1S/C9H6N2O3/c12-7(6-4-2-1-3-5-6)8-10-9(13)14-11-8/h1-5H,(H,10,11,13)
InchiKey: QVWHUXTXFTZSKG-UHFFFAOYSA-N
Formula: C9H6N2O3
SMILES: O=C(c1ccccc1)c1noc(O)n1
Mol. weight [g/mol]: 190.16
CAS: 30738-69-3

Physical Properties

Property code	Value	Unit	Source
chs	-4129.20 ± 7.90	kJ/mol	NIST Webbook
log10ws	-6.24		Crippen Method
logp	1.006		Crippen Method
mcvol	127.720	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30738693&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

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.