

1,2,4-Oxadiazol-3(2H)-one, 5-phenyl-

Other names: 1,2,4-Oxadiazol-3-ol, 5-phenyl-
Inchi: InChI=1S/C8H6N2O2/c11-8-9-7(12-10-8)6-4-2-1-3-5-6/h1-5H,(H,10,11)
InchiKey: INVHTFJJZGBKTM-UHFFFAOYSA-N
Formula: C8H6N2O2
SMILES: O=c1nc(-c2ccccc2)o[nH]1
Mol. weight [g/mol]: 162.15
CAS: 21084-84-4

Physical Properties

Property code	Value	Unit	Source
chs	-4001.20 ± 5.90	kJ/mol	NIST Webbook
log10ws	-6.22		Crippen Method
logp	0.548		Crippen Method
mcvol	112.060	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C21084844&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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