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

Other names: 3-phenyl-1,2,4-oxadiazol-5(4H)-one
Inchi: InChI=1S/C8H6N2O2/c11-8-9-7(10-12-8)6-4-2-1-3-5-6/h1-5H,(H,9,10,11)
InchiKey: LMBDRBXGTCUBIH-UHFFFAOYSA-N
Formula: C8H6N2O2
SMILES: O=c1[nH]c(-c2ccccc2)no1
Mol. weight [g/mol]: 162.15
CAS: 1456-22-0

Physical Properties

Property code	Value	Unit	Source
chs	-3896.10 ± 5.90	kJ/mol	NIST Webbook
log10ws	-6.22		Crippen Method
logp	0.548		Crippen Method
mcvol	112.060	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=C1456220&Units=SI

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