1,2,4-Oxadiazole, 3,5-diphenyl-

Other names: 3,5-Diphenyl-1,2,4-oxadiazole
Inchi: InChI=1S/C14H10N2O/c1-3-7-11(8-4-1)13-15-14(17-16-13)12-9-5-2-6-10-12/h1-10H
InchiKey: VIZNDSYPXQJMCM-UHFFFAOYSA-N
Formula: C14H10N2O
SMILES: c1ccc(-c2noc(-c3ccccc3)n2)cc1
Mol. weight [g/mol]: 222.24
CAS: 888-71-1

Physical Properties

Property code	Value	Unit	Source
chs	-7145.00 ± 11.00	kJ/mol	NIST Webbook
ie	9.20 ± 0.10	eV	NIST Webbook
log10ws	-9.94		Crippen Method
logp	3.404		Crippen Method
mcvol	166.970	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	483.20	K	2.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C888711&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure