4,5-Oxazoledione, 2-phenyl-, 4-phenylhydrazone

Inchi: InChI=1S/C15H11N3O2/c19-15-13(18-17-12-9-5-2-6-10-12)16-14(20-15)11-7-3-1-4-8-11

InchiKey: JGUNDRHHCZCUPV-QGOAFFKASA-N

Formula: C15H11N3O2

SMILES: O=C1OC(c2ccccc2)=NC1=NNc1ccccc1

Mol. weight [g/mol]: 265.27

CAS: 54506-04-6

Physical Properties

Property code	Value	Unit	Source
hf	143.03	kJ/mol	Joback Method
hvap	80.60	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.416		Crippen Method
mcvol	192.610	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
tb	897.85	K	Joback Method
tc	1183.82	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54506046&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature