

Oxazole, 2-methyl-4,5-diphenyl-

Other names:	2-Methyl-4,5-diphenyloxazole
Inchi:	InChI=1S/C16H13NO/c1-12-17-15(13-8-4-2-5-9-13)16(18-12)14-10-6-3-7-11-14/h2-11H,
InchiKey:	QLQIWRCWPJRJJA-UHFFFAOYSA-N
Formula:	C16H13NO
SMILES:	<chem>Cc1nc(-c2ccccc2)c(-c2ccccc2)o1</chem>
Mol. weight [g/mol]:	235.28
CAS:	14224-99-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.65		Crippen Method
logp	4.317		Crippen Method
mccvol	185.170	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	487.20	K	2.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14224998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcpvol: McGowan's characteristic volume
tbrp: Boiling point at reduced pressure

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