

Oxazole, 2-hexyl-4,5-dimethyl-

Other names:	2-Hexyl-4,5-dimethyl-1,3-oxazole 2-Hexyl-4,5-dimethyloxazole
Inchi:	InChI=1S/C11H19NO/c1-4-5-6-7-8-11-12-9(2)10(3)13-11/h4-8H2,1-3H3
InchiKey:	KNPWGHJHGHEJLW-UHFFFAOYSA-N
Formula:	C11H19NO
SMILES:	CCCCCCc1nc(C)c(C)o1
Mol. weight [g/mol]:	181.27
CAS:	20662-87-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.40		Crippen Method
logp	3.414		Crippen Method
mcvol	162.240	ml/mol	McGowan Method
rinpol	1287.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20662877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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