Oxazole, 4-methyl-2,5-dipropyl

Inchi: InChI=1S/C10H17NO/c1-4-6-9-8(3)11-10(12-9)7-5-2/h4-7H2,1-3H3
InchiKey: OGSRPIYHUJRQFZ-UHFFFAOYSA-N
Formula: C10H17NO
SMILES: CCCc1nc(C)c(CCC)o1
Mol. weight [g/mol]: 167.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.89		Crippen Method
logp	2.888		Crippen Method
mcvol	148.150	ml/mol	McGowan Method
rinpol	1159.00		NIST Webbook
ripol	1436.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R46182&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

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