

N-isoamyl(-) benzoxazolone

Inchi:	InChI=1S/C12H15NO2/c1-2-3-6-9-13-10-7-4-5-8-11(10)15-12(13)14/h4-5,7-8H,2-3,6,9H2
InchiKey:	PQWUXMAVMLAYBN-UHFFFAOYSA-N
Formula:	C12H15NO2
SMILES:	CCCCCn1c(=O)oc2ccccc21
Mol. weight [g/mol]:	205.25
CAS:	72548-10-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.95		Crippen Method
logp	2.785		Crippen Method
mcvol	162.740	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72548108&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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