

# Ethyl 3-bromo-4,6-dimethyl-2H-pyran-5-carboxylate

Other names:	3-Bromo-5-carbethoxy-4,6-dimethyl-2-pyrone 2H-Pyrane-5-carboxylic acid, 3-bromo-4,6-dimethyl-2-oxo-, ethyl ester
Inchi:	InChI=1S/C10H11BrO4/c1-4-14-9(12)7-5(2)8(11)10(13)15-6(7)3/h4H2,1-3H3
InchiKey:	YMOPMHLWTLUFGX-UHFFFAOYSA-N
Formula:	C10H11BrO4
SMILES:	CCOC(=O)c1c(C)oc(=O)c(Br)c1C
Mol. weight [g/mol]:	275.10
CAS:	18152-79-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.40		Crippen Method
logp	2.196		Crippen Method
mcvol	164.680	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C18152799&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18152799&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

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

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