3-Bromo-5-carbethoxy-4,6-dimethyl-2-pyrone

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

Physical Properties

Property code	Value	Unit	Source
ie	8.87	eV	Cheméo Relay (1.0)
logp	2.196		Crippen Method
mcvol	164.680	ml/mol	McGowan Method
tb	585.18	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18152799&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature