Coumarin, 3-formyl-4-methyl-7-(N,N-diethyl amino)-

Inchi: InChI=1S/C15H17NO3/c1-4-16(5-2)11-6-7-12-10(3)13(9-17)15(18)19-14(12)8-11/h6-9H,
InchiKey: ICAXYTLHINMBNG-UHFFFAOYSA-N
Formula: C15H17NO3
SMILES: CCN(CC)c1ccc2c(C)c(C=O)c(=O)oc2c1
Mol. weight [g/mol]: 259.30
CAS: 142730-48-1

Physical Properties

Property code	Value	Unit	Source
ie	7.64	eV	NIST Webbook
log10ws	-7.89		Crippen Method
logp	2.760		Crippen Method
mcvol	202.280	ml/mol	McGowan Method

Sources

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=C142730481&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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