7-Amino-4-(methoxymethyl)coumarin

Inchi: InChI=1S/C11H11NO3/c1-14-6-7-4-11(13)15-10-5-8(12)2-3-9(7)10/h2-5H,6,12H2,1H3
InchiKey: QZZLLHOMMCKWIQ-UHFFFAOYSA-N
Formula: C11H11NO3
SMILES: COCc1cc(=O)oc2cc(N)ccc12
Mol. weight [g/mol]: 205.21
CAS: 175205-10-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.45		Crippen Method
logp	1.522		Crippen Method
mcvol	150.220	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C175205104&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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