3-Acetamidocoumarin

Other names: 3-Acetamidocoumarin
Inchi: InChI=1S/C11H9NO3/c1-7(13)12-9-6-8-4-2-3-5-10(8)15-11(9)14/h2-6H,1H3,(H,12,13)
InchiKey: XJYLCCJIDYSFMB-UHFFFAOYSA-N
Formula: C11H9NO3
SMILES: CC(=O)Nc1cc2ccccc2oc1=O
Mol. weight [g/mol]: 203.20

Physical Properties

Property code	Value	Unit	Source
ie	8.58	eV	Cheméo Relay (1.0)
log10ws	-2.53		Cheméo Relay (1.0)
logp	1.751		Crippen Method
mcvol	145.920	ml/mol	McGowan Method
tb	619.17	K	Cheméo Relay (1.0)
tf	406.90	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C779306&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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