7-Amino-3-phenylcoumarin

Other names:	2H-1-Benzopyran-2-one, 7-amino-3-phenyl- 7-amino-3-phenyl-2-benzopyrone
Inchi:	InChI=1S/C15H11NO2/c16-12-7-6-11-8-13(10-4-2-1-3-5-10)15(17)18-14(11)9-12/h1-9H,
InchiKey:	IJCLOOKYCQWSJA-UHFFFAOYSA-N
Formula:	C15H11NO2
SMILES:	Nc1ccc2cc(-c3ccccc3)c(=O)oc2c1
Mol. weight [g/mol]:	237.25
CAS:	4108-61-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.67		Crippen Method
logp	3.042		Crippen Method
mcvol	176.950	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=C4108616&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.