

Coumarin, 3-(4-nitrophenyl)-

Inchi:	InChI=1S/C15H9NO4/c17-15-13(9-11-3-1-2-4-14(11)20-15)10-5-7-12(8-6-10)16(18)19/h
InchiKey:	GATDYELJYSMQPH-UHFFFAOYSA-N
Formula:	C15H9NO4
SMILES:	O=c1oc2ccccc2cc1-c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	267.24
CAS:	2555-25-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.69		Crippen Method
logp	3.368		Crippen Method
mcvol	184.390	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=C2555251&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

Latest version available from:

<https://www.chemeo.com/cid/91-251-2/Coumarin-3-4-nitrophenyl.pdf>

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