

1H-Naphtho[2,1-b]pyran-1-one, 3-phenyl-

Other names:	3-Phenyl-1H-naphtho(2,1-b)pyran-1-one 5,6-Benzoflavone «beta»-Naphthoflavone «beta»-Nf
Inchi:	InChI=1S/C19H12O2/c20-16-12-18(14-7-2-1-3-8-14)21-17-11-10-13-6-4-5-9-15(13)19(16)
InchiKey:	OUGIDAPQYNCXRA-UHFFFAOYSA-N
Formula:	C19H12O2
SMILES:	O=c1cc(-c2ccccc2)oc2ccc3ccccc3c12
Mol. weight [g/mol]:	272.30
CAS:	6051-87-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.84		Crippen Method
logp	4.613		Crippen Method
mcvol	203.870	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=C6051872&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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