Dimefline

Other names:	4H-1-Benzopyran-4-one, 8-[(dimethylamino)methyl]-7-methoxy-3-methyl-2-phenyl- Dimeflin Dimelfin Flavone, 8-((dimethylamino)methyl)-7-methoxy-3-methyl- Malivan N-(7-Methoxy-3-methyl-4-oxo-2-phenyl-4H-chromen-8-yl)methyl-N,N-dimethylamine Reanimil Remeflin 8-((Dimethylamino)methyl)-7-methoxy-3-methylflavone 8-((Dimethylamino)methyl)-7-methoxy-3-methyl-2-phenylchromone 3-Methyl-7-methoxy-8-[(dimethylamino)methyl]flavone NSC 169869
Inchi:	InChI=1S/C20H21NO3/c1-13-18(22)15-10-11-17(23-4)16(12-21(2)3)20(15)24-19(13)14-8
InchiKey:	ZXFQRFXLFWWKLX-UHFFFAOYSA-N
Formula:	C20H21NO3
SMILES:	COc1ccc2c(=O)c(C)c(-c3ccccc3)oc2c1CN(C)C
Mol. weight [g/mol]:	323.39
CAS:	1165-48-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.92		Crippen Method
logp	3.839		Crippen Method
mcvol	253.270	ml/mol	McGowan Method
rinpol	2679.00		NIST Webbook
rinpol	2660.00		NIST Webbook
rinpol	2685.00		NIST Webbook
rinpol	2660.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices