Irgacure 369 (2-Benzyl-2-(dimethylamino)-1-[4-(morpholinyl) phenyl)]-1-butanone)

Inchi: InChI=1S/C23H30N2O2/c1-4-23(24(2)3,18-19-8-6-5-7-9-19)22(26)20-10-12-21(13-11-20

InchiKey: UHFFVFAKEGKNAQ-UHFFFAOYSA-N

Formula: C23H30N2O2

SMILES: CCC(Cc1ccccc1)(C(=O)c1ccc(N2CCOCC2)cc1)N(C)C

Mol. weight [g/mol]: 366.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	3.659		Crippen Method
mcvol	303.950	ml/mol	McGowan Method
rinpol	3112.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R508486&Units=SI

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