

Irgacure 369

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

InChI: CC(C)(C(=O)C1=CC=C(C=C1)N(C)C)C2=CC=C(C=C2)N3CCOCC3
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
rinpole	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/ci9903071>
Crippen Method: https://www.cheméo.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
rinpole: Non-polar retention indices

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