

1-Propanone, 2-methyl-1-[4-(methylthio)phenyl]-2-(4-morpholinyl)

Other names:

2-Methyl-1-[4-(methylthio)phenyl]-2-morpholinopropanone-1

2-Methyl-1-[4-(methylthio)phenyl]-2-(4-morpholinyl)-1-propanone

Irgacure 907 (2-Methyl-1-(4-methyl thio) phenyl-2-(4-morpholinyl)-1-propanone)

Inchi:

InChI=1S/C15H21NO2S/c1-15(2,16-8-10-18-11-9-16)14(17)12-4-6-13(19-3)7-5-12/h4-7H

InchiKey:

LWRBVKNFOYUCNP-UHFFFAOYSA-N

Formula:

C₁₅H₂₁NO₂S

SMILES:

CSc1ccc(C(=O)C(C)(C)N2CCOCC2)cc1

Mol. weight [g/mol]:

279.40

CAS:

71868-10-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	2.702		Crippen Method
mcvol	221.360	ml/mol	McGowan Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C71868105&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
rinpol:	Non-polar retention indices

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