

Phthalimide, n-(p-methoxybenzyl)-

Inchi:	InChI=1S/C16H13NO3/c1-20-12-8-6-11(7-9-12)10-17-15(18)13-4-2-3-5-14(13)16(17)19/
InchiKey:	KBSAUETWMISGCC-UHFFFAOYSA-N
Formula:	C16H13NO3
SMILES:	COc1ccc(CN2C(=O)c3ccccc3C2=O)cc1
Mol. weight [g/mol]:	267.28
CAS:	21244-24-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.06		Crippen Method
logp	2.491		Crippen Method
mcvol	196.910	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21244246&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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<https://www.chemeo.com/cid/46-587-0/Phthalimide-n-p-methoxybenzyl.pdf>

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