N-Benzylmaleimide

Other names:	1H-Pyrrole-2,5-dione, 1-(phenylmethyl)-
	1-benzyl-1H-pyrrole-2,5-dione
Inchi:	InChI=1S/C11H9NO2/c13-10-6-7-11(14)12(10)8-9-4-2-1-3-5-9/h1-7H,8H2
InchiKey:	MKRBAPNEJMFMHU-UHFFFAOYSA-N
Formula:	C11H9NO2
SMILES:	O=C1C=CC(=O)N1Cc1ccccc1
Mol. weight [g/mol]:	187.19
CAS:	1631-26-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.89		Crippen Method
logp	1.112		Crippen Method
mcvol	140.050	ml/mol	McGowan Method

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1631261&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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