2,5-Pyrrolidinedione, 1-(phenylmethyl)-

Other names:	Pyrrolidine-2,5-dione, 1-(phenylmethyl)- Pyrrolidine-2,5-dione, 1-benzyl- N-Benzylsuccinimide
Inchi:	InChI=1S/C11H11NO2/c13-10-6-7-11(14)12(10)8-9-4-2-1-3-5-9/h1-5H,6-8H2
InchiKey:	IONNJVQITCVNHK-UHFFFAOYSA-N
Formula:	C11H11NO2
SMILES:	O=C1CCC(=O)N1Cc1ccccc1
Mol. weight [g/mol]:	189.21
CAS:	2142-06-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	1.336		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
rinpol	1708.50		NIST Webbook
rinpol	1708.50		NIST Webbook

Sources

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=C2142065&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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