

PYRROLO[1,2-A]PYRAZINE-1,4-DIONE, HEXAHYDRO-3-(PHENYLMETHYL)-

Other names:	Cyclo-Phe-Pro-diketopiperazine
Inchi:	InChI=1S/C14H16N2O2/c17-13-12-7-4-8-16(12)14(18)11(15-13)9-10-5-2-1-3-6-10/h1-3,5
InchiKey:	QZBUWPVZSXDWSB-UHFFFAOYSA-N
Formula:	C14H16N2O2
SMILES:	O=C1NC(Cc2ccccc2)C(=O)N2CCCC12
Mol. weight [g/mol]:	244.29

Physical Properties

Property code	Value	Unit	Source
logp	0.718		Crippen Method
mcvol	185.740	ml/mol	McGowan Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14705603&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/113-394-9/PYRROLO-1-2-A-PYRAZINE-1-4-DIONE-HEXAHYDRO-3-PHENYLMETHYL>

Generated by Cheméo on 2026-07-21 12:24:38.429859513 +0000 UTC m=+147774.271744902.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.