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
CAS: 14705-60-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14705603&Units=SI

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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