

Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-

Other names: Hexahydropyrrolo[1,2-a]pyrazine-1,4-dione
Pyrrolidino[1,2-a]piperazine-3,6-dione

Inchi: InChI=1S/C7H10N2O2/c10-6-4-8-7(11)5-2-1-3-9(5)6/h5H,1-4H2,(H,8,11)

InchiKey: OWOHLURDBZHNGG-UHFFFAOYSA-N

Formula: C7H10N2O2

SMILES: O=C1NCC(=O)N2CCCC12

Mol. weight [g/mol]: 154.17

CAS: 19179-12-5

Physical Properties

Property code	Value	Unit	Source
log10ws	0.04		Crippen Method
logp	-0.893		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
rinpol	1795.20		NIST Webbook
rinpol	1795.20		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C19179125&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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