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/ci990307l
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