1,4-Piperazinedicarboxamide, 2-methyl-

Inchi: InChI=1S/C7H14N4O2/c1-5-4-10(6(8)12)2-3-11(5)7(9)13/h5H,2-4H2,1H3,(H2,8,12)(H2,9

InchiKey: NRCCTZFBDCDAPP-UHFFFAOYSA-N

Formula: C7H14N4O2

SMILES: CC1CN(C(N)=O)CCN1C(N)=O

Mol. weight [g/mol]: 186.21

CAS: 116594-99-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.27		Crippen Method
logp	-0.850		Crippen Method
mcvol	141.690	ml/mol	McGowan Method

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=C116594991&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume