

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

Latest version available from:

<https://www.chemeo.com/cid/39-747-0/1-4-Piperazinedicarboxamide-2-methyl.pdf>

Generated by Cheméo on 2025-12-25 00:36:23.209845763 +0000 UTC m=+6371180.739886417.

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