

Imidazo[4,5-d]imidazole-2,5-(1H,3H)dione, tetrahydro-1,3,4,6-tetramethyl-

Other names:	1,3,4,6-tetramethylglycoluril 2,4,6,8-Tetraazabicyclo[3.3.0]octane-3,7-dione, 2,4,6,8-tetramethyl-Mebicar glycoluril, 1,3,4,6-tetramethyl-imidazo[4,5-d]imidazole-2,5(1H,3H)-dione, tetrahydro-1,3,4,6-tetramethyl-tetrahydro-1,3,4,6-tetramethylimidazo(4,5-d)imidazole-2,5(1H,3H)-dione
Inchi:	InChI=1S/C8H14N4O2/c1-9-5-6(11(3)7(9)13)12(4)8(14)10(5)2/h5-6H,1-4H3
InchiKey:	XIUUSFJTJXFNGH-UHFFFAOYSA-N
Formula:	C8H14N4O2
SMILES:	CN1C(=O)N(C)C2C1N(C)C(=O)N2C
Mol. weight [g/mol]:	198.22
CAS:	10095-06-4

Physical Properties

Property code	Value	Unit	Source
log10ws	0.04		Crippen Method
logp	-0.367		Crippen Method
mcpvol	144.920	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C10095064&Units=SI>

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

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

Enthalpy-related interaction parameters in H/D isotopically distinguishable <https://www.doi.org/10.1016/j.tca.2011.05.019>

McGowan Method of tetramethylurea cyclic derivatives at 298.15 K: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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