Sarcosine anhydride

Other names:	1,4-Dimethyl-2,5-dioxopiperazine
	1,4-Dimethylpiperazine-2,5-dione
	1,4-Dimethylpiperazine-2,5-dione (chcl3 solution)
	1,4-Dimethylpiperazine-2,5-dione (oil mull)
	1,4-dimethyl-2,5-piperazinedione
	2,5-Piperazinedione, 1,4-dimethyl-
	Cyclo(sarcosylsarcosyl)
	N,N'-Dimethyldiketopiperazine
	NSC 67461
	Sarcosine anhydride, bimol. cyclic
	Sarcosine diketopiperazine
Inchi:	InChI=1S/C6H10N2O2/c1-7-3-6(10)8(2)4-5(7)9/h3-4H2,1-2H3
InchiKey:	PKDGRAULLDDTRN-UHFFFAOYSA-N
Formula:	C6H10N2O2
SMILES:	CN1CC(=O)N(C)CC1=O
Mol. weight [g/mol]:	142.16
CAS:	5076-82-4

Physical Properties

Property code	Value	Unit	Source
log10ws	1.08		Crippen Method
logp	-1.083		Crippen Method
mcvol	107.640	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	103.60	kJ/mol	298.15	Thermochemistry of sarcosine and sarcosine anhydride: Theoretical and experimental studies

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5076824&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Thermochemistry of sarcosine and sarcosine anhydride: Theoretical and experimental studies: https://www.doi.org/10.1016/j.jct.2012.11.019

Legend

hvapt: Enthalpy of vaporization at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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