5,5'-Methylene-bis(2-keto-1,3-dimethyltetrahydro-

Inchi: InChI=1S/C11H22N6O2/c1-12-5-16(6-13(2)10(12)18)9-17-7-14(3)11(19)15(4)8-17/h5-9H
InchiKey: VLJFBQORFVZBSR-UHFFFAOYSA-N
Formula: C11H22N6O2
SMILES: CN1CN(CN2CN(C)C(=O)N(C)C2)CN(C)C1=O
Mol. weight [g/mol]: 270.33
CAS: 126591-36-4

Physical Properties

Property code	Value	Unit	Source
chs	-7078.30 ± 3.30	kJ/mol	NIST Webbook
hfs	-394.40 ± 3.30	kJ/mol	NIST Webbook
log10ws	0.38		Crippen Method
logp	-0.628		Crippen Method
mcvol	207.150	ml/mol	McGowan Method

Sources

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=C126591364&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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