

N'-(2,7-Dioxooxepan-3-yl)-N,N-dimethylimidoform

Inchi: InChI=1S/C9H14N2O3/c1-11(2)6-10-7-4-3-5-8(12)14-9(7)13/h6-7H,3-5H2,1-2H3
InchiKey: YAMSMQZMXXMHSC-UHFFFAOYSA-N
Formula: C9H14N2O3
SMILES: CN(C)C=NC1CCCC(=O)OC1=O
Mol. weight [g/mol]: 198.22

Physical Properties

Property code	Value	Unit	Source
hf	-438.58	kJ/mol	Joback Method
hvap	54.59	kJ/mol	Joback Method
log10ws	-0.46		Crippen Method
logp	0.199		Crippen Method
mcvol	151.480	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpola	1691.00		NIST Webbook
rinpola	1691.00		NIST Webbook
tb	680.85	K	Joback Method
tc	929.37	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375708&Units=SI>

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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