

Biuret, 1-methyl-1-nitroso-

Inchi: InChI=1S/C3H6N4O3/c1-7(6-10)3(9)5-2(4)8/h1H3,(H3,4,5,8,9)
InchiKey: YBODEWRZWWTHPL-UHFFFAOYSA-N
Formula: C3H6N4O3
SMILES: CN(N=O)C(O)=NC(=N)O
Mol. weight [g/mol]: 146.10
CAS: 13860-69-0

Physical Properties

Property code	Value	Unit	Source
hf	-239.61	kJ/mol	Joback Method
hvap	82.25	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	0.006		Crippen Method
mcvol	97.760	ml/mol	McGowan Method
tb	689.14	K	Joback Method

Sources

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=C13860690&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

tb: Normal Boiling Point Temperature

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