

Urea], 1,1'-trimethylenebis[3-methyl-3-nitroso-

Inchi: InChI=1S/C7H14N6O4/c1-12(10-16)6(14)8-4-3-5-9-7(15)13(2)11-17/h3-5H2,1-2H3,(H,8,
InchiKey: VNYXNTQYEYQRCJ-UHFFFAOYSA-N
Formula: C7H14N6O4
SMILES: CN(N=O)C(=O)NCCCNC(=O)N(C)N=O
Mol. weight [g/mol]: 246.22
CAS: 13404-51-8

Physical Properties

Property code	Value	Unit	Source
hf	-507.35	kJ/mol	Joback Method
hvap	79.82	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	0.022		Crippen Method
mcvol	175.650	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
tb	719.32	K	Joback Method
tc	905.32	K	Joback Method

Sources

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=C13404518&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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