

Biurea, 1,6-dimethyl-1,6-dinitroso-

Inchi:	InChI=1S/C4H8N6O4/c1-9(7-13)3(11)5-6-4(12)10(2)8-14/h1-2H3,(H,5,11)(H,6,12)
InchiKey:	VWCDVSANFVCUOI-UHFFFAOYSA-N
Formula:	C4H8N6O4
SMILES:	CN(N=O)C(O)=NN=C(O)N(C)N=O
Mol. weight [g/mol]:	204.14
CAS:	3844-60-8

Physical Properties

Property code	Value	Unit	Source
hf	-486.81	kJ/mol	Joback Method
hvap	86.92	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	-0.044		Crippen Method
mcvol	133.380	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
tb	780.08	K	Joback Method
tc	971.69	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=C3844608&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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