1,3,5-Trinitroso-1,3,5-triazacyclohexane

Inchi:	InChI=1S/C3H6N6O3/c10-7-1-4-2(8-11)6-3(5-1)9-12/h10-12H,(H3,4,5,6,7,8,9)
InchiKey:	FZVSRQPFVSOCAU-UHFFFAOYSA-N
Formula:	C3H6N6O3
SMILES:	ONc1nc(NO)nc(NO)n1
Mol. weight [g/mol]:	174.12
CAS:	23374-70-1

Physical Properties

Property code	Value	Unit	Source
log10ws	1.50		Crippen Method
logp	-0.725		Crippen Method
mcvol	106.860	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23374701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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