

# 2,4,7-Trinitroanthren-9-one

<b>Other names:</b>	2,4,7-Trinitroanthrone
<b>Inchi:</b>	InChI=1S/C13H5N3O8/c17-12-8-3-6(14(18)19)1-2-11(8)24-13-9(12)4-7(15(20)21)5-10(1
<b>InchiKey:</b>	GRKGPRVKUQAYIM-UHFFFAOYSA-N
<b>Formula:</b>	C13H5N3O8
<b>SMILES:</b>	O=c1c2cc([N+](=O)[O-])ccc2oc2c([N+](=O)[O-])cc([N+](=O)[O-])cc12
<b>Mol. weight [g/mol]:</b>	331.19
<b>CAS:</b>	131032-92-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.19		Crippen Method
logp	2.671		Crippen Method
mccvol	195.350	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	31.40	kJ/mol	477.80	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C131032923&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C131032923&amp;Units=SI</a>

## Legend

**hfust:** Enthalpy of fusion at a given temperature  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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