

# 4,7,13,16-Tetraoxa-1,10-dithiacyclooctadecane-1,10-dithione (alpha-form)

InChI: Cc1ccc(S(=O)(=O)N=S2CCOCCOCCS(=NS(=O)(=O)c3ccc(C)cc3)CCOCCOCC2)cc1  
InChIKey: BTNZQMNKMYFQLK-UHFFFAOYSA-N  
Formula: C<sub>26</sub>H<sub>38</sub>N<sub>2</sub>O<sub>8</sub>S<sub>4</sub>  
SMILES: Cc1ccc(S(=O)(=O)N=S2CCOCCOCCS(=NS(=O)(=O)c3ccc(C)cc3)CCOCCOCC2)cc1  
Mol. weight [g/mol]: 634.85  
CAS: 119698-57-6

## Physical Properties

Property code	Value	Unit	Source
hf	-1537.69	kJ/mol	Joback Method
hvap	156.05	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	3.065		Crippen Method
mcvol	451.140	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
tb	1382.68	K	Joback Method
tc	1695.55	K	Joback Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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=C119698576&Units=SI&Mask=3FFF>  
**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

<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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