

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

InChI: InChI=1S/C26H38N2O8S4/c1-23-3-7-25(8-4-23)39(29,30)27-37-19-15-33-11-13-35-17-2  
InChIKey: BTNZQMNKMYFQLK-UHFFFAOYSA-N  
Formula: C26H38N2O8S4  
SMILES: Cc1ccc(S(=O)(=O)N=S2CCOCCOCCS(=NS(=O)(=O)c3ccc(C)cc3)CCOCCOCC2)cc1  
Mol. weight [g/mol]: 634.85

## 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

**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=B6002154&Units=SI&Mask=3FFF>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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