4,7,13,16-Tetraoxa-1,10-dithiacyclooctadecane-1,1 (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
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/ci990307l
Crippen Method: 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