4,10-Dioxa-1,7-dithiacyclododecane, 1,1,7,7-tetraoxide

Inchi: InChI=1S/C8H16O6S2/c9-15(10)5-1-13-2-6-16(11,12)8-4-14-3-7-15/h1-8H2
InchiKey: OPRRNWDOIKQGOP-UHFFFAOYSA-N
Formula: C8H16O6S2
SMILES: O=S1(=O)CCOCCS(=O)(=O)CCOCC1
Mol. weight [g/mol]: 272.34
CAS: 98561-09-2

Physical Properties

Property code	Value	Unit	Source
gf	-1119.80	kJ/mol	Joback Method
hf	-1334.67	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	79.45	kJ/mol	Joback Method
log10ws	1.09		Crippen Method
logp	-1.137		Crippen Method
mcvol	180.640	ml/mol	McGowan Method
pc	5470.75	kPa	Joback Method
tb	539.84	K	Joback Method
tc	756.94	K	Joback Method
tf	398.78	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.27	J/mol×K	539.84	Joback Method
cpg	449.30	J/mol×K	576.02	Joback Method
cpg	469.16	J/mol×K	612.21	Joback Method
cpg	487.79	J/mol×K	648.39	Joback Method
cpg	505.17	J/mol×K	684.57	Joback Method
cpg	521.27	J/mol×K	720.76	Joback Method
cpg	536.04	J/mol×K	756.94	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C98561092&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume