4,7,13,16-Tetraoxa-1,10-dithiacyclooctadecane

Other names: 1,4,10,13-tetraoxa-7,16-dithiacyclooctadecane
Inchi: InChI=1S/C12H24O4S2/c1-2-14-6-10-18-12-8-16-4-3-15-7-11-17-9-5-13-1/h1-12H2
InchiKey: LIQFCELSAWJXJN-UHFFFAOYSA-N
Formula: C12H24O4S2
SMILES: C1COCCSCCOCCOCCSCCO1
Mol. weight [g/mol]: 296.45
CAS: 296-39-9

Physical Properties

Property code	Value	Unit	Source
gf	-327.64	kJ/mol	Joback Method
hf	-727.75	kJ/mol	Joback Method
hfus	31.63	kJ/mol	Joback Method
hvap	74.77	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	1.533		Crippen Method
mcvol	225.260	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	752.88	K	Joback Method
tc	1053.38	K	Joback Method
tf	467.56	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.77	J/mol×K	752.88	Joback Method
cpg	700.95	J/mol×K	802.96	Joback Method
cpg	723.67	J/mol×K	853.05	Joback Method
cpg	742.78	J/mol×K	903.13	Joback Method
cpg	758.13	J/mol×K	953.22	Joback Method
cpg	769.56	J/mol×K	1003.30	Joback Method
cpg	776.92	J/mol×K	1053.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C296399&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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