1,7-Dioxa-4,10-dithiacyclododecane

Other names: 4,10-Dioxa-1,7-dithiacyclododecane
Inchi: InChI=1S/C8H16O2S2/c1-5-11-7-3-10-4-8-12-6-2-9-1/h1-8H2
InchiKey: ANWGCVKFPKDUBI-UHFFFAOYSA-N
Formula: C8H16O2S2
SMILES: C1CSCCOCCSCCO1
Mol. weight [g/mol]: 208.34
CAS: 294-95-1

Physical Properties

Property code	Value	Unit	Source
gf	-116.48	kJ/mol	Joback Method
hf	-344.23	kJ/mol	Joback Method
hfus	17.91	kJ/mol	Joback Method
hvap	55.82	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	1.500		Crippen Method
mcvol	157.160	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	1681.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1742.90		NIST Webbook
tb	581.84	K	Joback Method
tc	864.43	K	Joback Method
tf	390.46	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.51	J/mol×K	581.84	Joback Method
cpg	398.96	J/mol×K	628.94	Joback Method
cpg	419.69	J/mol×K	676.04	Joback Method
cpg	438.67	J/mol×K	723.14	Joback Method

cpg	455.85	J/mol×K	770.23	Joback Method
cpg	471.22	J/mol×K	817.33	Joback Method
cpg	484.72	J/mol×K	864.43	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C294951&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume