4,7,10-Trioxa-1-thiacyclododecane

Inchi: InChI=1S/C8H16O3S/c1-3-10-5-7-12-8-6-11-4-2-9-1/h1-8H2
InchiKey: JMPKDBRUIAOFAO-UHFFFAOYSA-N
Formula: C8H16O3S
SMILES: C1COCCSCCOCCO1
Mol. weight [g/mol]: 192.28
CAS: 294-94-0

Physical Properties

Property code	Value	Unit	Source
gf	-242.46	kJ/mol	Joback Method
hf	-521.49	kJ/mol	Joback Method
hfus	22.23	kJ/mol	Joback Method
hvap	54.51	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	0.783		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	560.96	K	Joback Method
tc	826.14	K	Joback Method
tf	333.58	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.92	J/mol×K	560.96	Joback Method
cpg	380.86	J/mol×K	605.16	Joback Method
cpg	401.30	J/mol×K	649.35	Joback Method
cpg	420.22	J/mol×K	693.55	Joback Method
cpg	437.56	J/mol×K	737.74	Joback Method
cpg	453.30	J/mol×K	781.94	Joback Method
cpg	467.38	J/mol×K	826.14	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=C294940&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