1,7-Dioxa-4,10-13-trithiacyclopentadecane

Inchi: InChI=1S/C10H20O2S3/c1-5-13-6-2-12-4-8-15-10-9-14-7-3-11-1/h1-10H2
InchiKey: SOEJNDLYEVYFIB-UHFFFAOYSA-N
Formula: C10H20O2S3
SMILES: C1CSCCOCCSCCSCCO1
Mol. weight [g/mol]: 268.46

Physical Properties

Property code	Value	Unit	Source
gf	-96.08	kJ/mol	Joback Method
hf	-358.73	kJ/mol	Joback Method
hfus	20.45	kJ/mol	Joback Method
hvap	66.60	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	2.233		Crippen Method
mcvol	201.690	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
rinpol	2172.00		NIST Webbook
rinpol	2257.10		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2172.00		NIST Webbook
tb	688.24	K	Joback Method
tc	998.59	K	Joback Method
tf	485.89	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.20	J/mol×K	688.24	Joback Method
cpg	562.87	J/mol×K	739.96	Joback Method
cpg	585.75	J/mol×K	791.69	Joback Method
cpg	605.74	J/mol×K	843.41	Joback Method
cpg	622.75	J/mol×K	895.14	Joback Method
cpg	636.69	J/mol×K	946.86	Joback Method

cpg	647.45	J/mol×K	998.59	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=R41445&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