1,10-Dioxa-4,7,13,16-tetrathiacyclooctadecane

Inchi: InChI=1S/C12H24O2S4/c1-5-15-9-10-17-7-3-14-4-8-18-12-11-16-6-2-13-1/h1-12H2
InchiKey: BFVXNKXLPBNMQI-UHFFFAOYSA-N
Formula: C12H24O2S4
SMILES: C1CSCCSCCOCCSCCSCCO1
Mol. weight [g/mol]: 328.58
CAS: 296-40-2

Physical Properties

Property code	Value	Unit	Source
gf	-75.68	kJ/mol	Joback Method
hf	-373.23	kJ/mol	Joback Method
hfus	22.99	kJ/mol	Joback Method
hvap	77.38	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.966		Crippen Method
mcvol	246.220	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
rinpol	2833.00		NIST Webbook
tb	794.64	K	Joback Method
tc	1128.14	K	Joback Method
tf	581.32	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.89	J/mol×K	794.64	Joback Method
cpg	735.46	J/mol×K	850.22	Joback Method
cpg	756.75	J/mol×K	905.81	Joback Method
cpg	773.58	J/mol×K	961.39	Joback Method
cpg	785.77	J/mol×K	1016.97	Joback Method
cpg	793.15	J/mol×K	1072.56	Joback Method
cpg	795.53	J/mol×K	1128.14	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=C296402&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