2,4,5,7-Tetrathiaoctane 2-oxide

Inchi: InChI=1S/C4H10OS4/c1-6-3-7-8-4-9(2)5/h3-4H2,1-2H3
InchiKey: VPVZUGOYFPCRCQ-UHFFFAOYSA-N
Formula: C4H10OS4
SMILES: CSCSSCS(C)=O
Mol. weight [g/mol]: 202.38
CAS: 155994-66-4

Physical Properties

Property code	Value	Unit	Source
gf	-135.55	kJ/mol	Joback Method
hf	-206.02	kJ/mol	Joback Method
hfus	26.26	kJ/mol	Joback Method
hvap	57.67	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	2.024		Crippen Method
mcvol	138.490	ml/mol	McGowan Method
pc	4659.34	kPa	Joback Method
rinpol	1813.50		NIST Webbook
rinpol	1813.50		NIST Webbook
tb	555.54	K	Joback Method
tc	803.89	K	Joback Method
tf	274.52	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.13	J/mol×K	555.54	Joback Method
cpg	285.14	J/mol×K	596.93	Joback Method
cpg	295.53	J/mol×K	638.32	Joback Method
cpg	305.24	J/mol×K	679.71	Joback Method
cpg	314.24	J/mol×K	721.11	Joback Method
cpg	322.48	J/mol×K	762.50	Joback Method
cpg	329.94	J/mol×K	803.89	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=C155994664&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume