2,3,5-trithiahexane 5-oxide

Inchi: InChI=1S/C3H8OS3/c1-5-6-3-7(2)4/h3H2,1-2H3
InchiKey: PVUZSKRNQWELBA-UHFFFAOYSA-N
Formula: C3H8OS3
SMILES: CSSCS(C)=O
Mol. weight [g/mol]: 156.29
CAS: 42474-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-177.09	kJ/mol	Joback Method
hf	-227.25	kJ/mol	Joback Method
hfus	19.54	kJ/mol	Joback Method
hvap	48.63	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	1.334		Crippen Method
mcvol	108.050	ml/mol	McGowan Method
pc	5205.63	kPa	Joback Method
rinpol	1395.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1408.00		NIST Webbook
tb	463.88	K	Joback Method
tc	694.15	K	Joback Method
tf	228.85	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.14	J/mol×K	463.88	Joback Method
cpg	201.06	J/mol×K	502.26	Joback Method
cpg	209.63	J/mol×K	540.64	Joback Method
cpg	217.81	J/mol×K	579.01	Joback Method
cpg	225.58	J/mol×K	617.39	Joback Method

cpg	232.93	J/mol×K	655.77	Joback Method
cpg	239.81	J/mol×K	694.15	Joback Method

Sources

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=C42474271&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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