2,4,5-trithiahexane 2,2-dioxide

Inchi: InChI=1S/C3H8O2S3/c1-6-7-3-8(2,4)5/h3H2,1-2H3
InchiKey: LFWLERCUMIQJQV-UHFFFAOYSA-N
Formula: C3H8O2S3
SMILES: CSSCS(C)(=O)=O
Mol. weight [g/mol]: 172.29
CAS: 42474-28-2

Physical Properties

Property code	Value	Unit	Source
gf	-427.92	kJ/mol	Joback Method
hf	-474.86	kJ/mol	Joback Method
hfus	23.16	kJ/mol	Joback Method
hvap	54.54	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.000		Crippen Method
mcvol	113.920	ml/mol	McGowan Method
pc	5765.39	kPa	Joback Method
rinpol	1452.80		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1452.80		NIST Webbook
tb	453.38	K	Joback Method
tc	667.63	K	Joback Method
tf	230.93	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.30	J/mol×K	453.38	Joback Method
cpg	215.40	J/mol×K	489.09	Joback Method
cpg	224.17	J/mol×K	524.80	Joback Method
cpg	232.57	J/mol×K	560.50	Joback Method
cpg	240.59	J/mol×K	596.21	Joback Method

cpg	248.20	J/mol×K	631.92	Joback Method
cpg	255.37	J/mol×K	667.63	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=C42474282&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