2,4-Dithiapentane 2,2-dioxide

Inchi: InChI=1S/C3H8O2S2/c1-6-3-7(2,4)5/h3H2,1-2H3
InchiKey: MPHBIACXKTZAFW-UHFFFAOYSA-N
Formula: C3H8O2S2
SMILES: CSCS(C)(=O)=O
Mol. weight [g/mol]: 140.22
CAS: 20163-71-7

Physical Properties

Property code	Value	Unit	Source
gf	-461.04	kJ/mol	Joback Method
hf	-516.73	kJ/mol	Joback Method
hfus	19.03	kJ/mol	Joback Method
hvap	47.72	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	0.352		Crippen Method
mcvol	97.570	ml/mol	McGowan Method
pc	5619.38	kPa	Joback Method
rinpol	1203.70		NIST Webbook
rinpol	1203.70		NIST Webbook
tb	384.60	K	Joback Method
tc	573.93	K	Joback Method
tf	196.53	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.11	J/mol×K	384.60	Joback Method
cpg	174.25	J/mol×K	416.15	Joback Method
cpg	182.16	J/mol×K	447.71	Joback Method
cpg	189.83	J/mol×K	479.26	Joback Method
cpg	197.23	J/mol×K	510.82	Joback Method
cpg	204.37	J/mol×K	542.37	Joback Method
cpg	211.23	J/mol×K	573.93	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=C20163717&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