1,3-Dithiolane-1,1,3,3-tetraoxide

Inchi: InChI=1S/C3H6O4S2/c4-8(5)1-2-9(6,7)3-8/h1-3H2
InchiKey: DQLOTKZORORBPO-UHFFFAOYSA-N
Formula: C3H6O4S2
SMILES: O=S1(=O)CCS(=O)(=O)C1
Mol. weight [g/mol]: 170.21
CAS: 26413-19-4

Physical Properties

Property code	Value	Unit	Source
gf	-904.96	kJ/mol	Joback Method
hf	-924.35	kJ/mol	Joback Method
hfus	18.20	kJ/mol	Joback Method
hvap	58.10	kJ/mol	Joback Method
log10ws	0.86		Crippen Method
logp	-1.213		Crippen Method
mcvol	98.450	ml/mol	McGowan Method
pc	9444.29	kPa	Joback Method
tb	341.65	K	Joback Method
tc	514.89	K	Joback Method
tf	313.93	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.50	J/mol×K	341.65	Joback Method
cpg	169.58	J/mol×K	370.52	Joback Method
cpg	179.21	J/mol×K	399.40	Joback Method
cpg	188.41	J/mol×K	428.27	Joback Method
cpg	197.17	J/mol×K	457.15	Joback Method
cpg	205.51	J/mol×K	486.02	Joback Method
cpg	213.43	J/mol×K	514.89	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=C26413194&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume