1,4-Dithiane-1-oxide

Other names: p-Dithiane, 1-oxide
1,4-Dithiacyclohexane 1-oxide
Inchi: InChI=1S/C4H8OS2/c5-7-3-1-6-2-4-7/h1-4H2
InchiKey: VBDLSQFQIUGPSA-UHFFFAOYSA-N
Formula: C4H8OS2
SMILES: O=S1CCSCC1
Mol. weight [g/mol]: 136.24
CAS: 19087-70-8

Physical Properties

Property code	Value	Unit	Source
gf	-156.15	kJ/mol	Joback Method
hf	-208.32	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	42.77	kJ/mol	Joback Method
log10ws	0.09		Crippen Method
logp	0.482		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
pc	5853.95	kPa	Joback Method
tb	400.30	K	Joback Method
tc	628.72	K	Joback Method
tf	315.44	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.55	J/mol×K	400.30	Joback Method
cpg	170.82	J/mol×K	438.37	Joback Method
cpg	182.34	J/mol×K	476.44	Joback Method
cpg	193.14	J/mol×K	514.51	Joback Method
cpg	203.24	J/mol×K	552.58	Joback Method
cpg	212.67	J/mol×K	590.65	Joback Method
cpg	221.45	J/mol×K	628.72	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=C19087708&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume