1,3-DITHIANE, 1-OXIDE

Other names: 1,3-Dithiane, 1-oxide
1,3-Dithiane sulfoxide
Inchi: InChI=1S/C4H8OS2/c5-7-3-1-2-6-4-7/h1-4H2
InchiKey: ONTCBWKSXDATLL-UHFFFAOYSA-N
Formula: C4H8OS2
SMILES: O=S1CCCSC1
Mol. weight [g/mol]: 136.24

Physical Properties

Property code	Value	Unit	Source
hfus	7.82	kJ/mol	Joback Method
ie	8.56	eV	Cheméo Relay (1.0)
logp	0.830		Crippen Method
mcvol	94.930	ml/mol	McGowan 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
hfust	22.60	kJ/mol	361.90	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16487108&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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