2-Methyl-1,4-dithiane

Other names: 1,4-Dithiane, methyl
1,4-Dithian, methyl
Inchi: InChI=1S/C5H10S2/c1-5-4-6-2-3-7-5/h5H,2-4H2,1H3
InchiKey: JMDYHOLGUWKACX-UHFFFAOYSA-N
Formula: C5H10S2
SMILES: CC1CSCCS1
Mol. weight [g/mol]: 134.26

Physical Properties

Property code	Value	Unit	Source
gf	95.39	kJ/mol	Joback Method
hf	-1.69	kJ/mol	Joback Method
hfus	7.85	kJ/mol	Joback Method
hvap	38.78	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.855		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
rinpol	1138.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tb	429.01	K	Joback Method
tc	672.02	K	Joback Method
tf	320.39	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.03	J/mol×K	429.01	Joback Method
cpg	199.05	J/mol×K	469.51	Joback Method
cpg	212.21	J/mol×K	510.01	Joback Method

cpg	224.55	J/mol×K	550.52	Joback Method
cpg	236.10	J/mol×K	591.02	Joback Method
cpg	246.88	J/mol×K	631.52	Joback Method
cpg	256.93	J/mol×K	672.02	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=R125794&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