1,3-Dithiane, 2-methyl-

Other names:	m-Dithiane, 2-methyl-
	2-Methyl-1,3-dithiane
	2-Methyl-m-dithiane
	Methyl-2 dithiane-1,3
	Acetaldehyde, cyclic trimethylene mercaptal
Inchi:	InChI=1S/C5H10S2/c1-5-6-3-2-4-7-5/h5H,2-4H2,1H3
InchiKey:	KXROTPXCYDXGSC-UHFFFAOYSA-N
Formula:	C5H10S2
SMILES:	CC1SCCCS1
Mol. weight [g/mol]:	134.26
CAS:	6007-26-7

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	-2.18		Crippen Method
logp	2.202		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
rinpol	1033.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1023.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1476.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	330.70	K	0.40	NIST Webbook

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=C6007267&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume