1,3-Dithiane, 2,2-dimethyl-

Other names: m-Dithiane, 2,2-dimethyl-
2,2-Dimethyl-1,3-dithiane
Inchi: InChI=1S/C6H12S2/c1-6(2)7-4-3-5-8-6/h3-5H2,1-2H3
InchiKey: YRFVUSVRBICMRJ-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CC1(C)SCCCS1
Mol. weight [g/mol]: 148.29
CAS: 6007-22-3

Physical Properties

Property code	Value	Unit	Source
gf	98.32	kJ/mol	Joback Method
hf	-7.09	kJ/mol	Joback Method
hfus	4.15	kJ/mol	Joback Method
hvap	39.85	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.593		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
tb	452.13	K	Joback Method
tc	702.61	K	Joback Method
tf	355.56	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.83	J/mol×K	452.13	Joback Method
cpg	241.41	J/mol×K	493.88	Joback Method
cpg	255.67	J/mol×K	535.62	Joback Method
cpg	268.76	J/mol×K	577.37	Joback Method
cpg	280.85	J/mol×K	619.12	Joback Method
cpg	292.11	J/mol×K	660.86	Joback Method
cpg	302.72	J/mol×K	702.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6007223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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