1,3-Dithiane

Other names: m-Dithiane
1,3-Dithiacyclohexane
Dithiane-1,3
Inchi: InChI=1S/C4H8S2/c1-2-5-4-6-3-1/h1-4H2
InchiKey: WQADWIOXOXRPLN-UHFFFAOYSA-N
Formula: C4H8S2
SMILES: C1CSCSC1
Mol. weight [g/mol]: 120.24
CAS: 505-23-7

Physical Properties

Property code	Value	Unit	Source
gf	94.68	kJ/mol	Joback Method
hf	39.29	kJ/mol	Joback Method
hfus	4.19	kJ/mol	Joback Method
hsub	52.30 ± 0.80	kJ/mol	NIST Webbook
hsub	62.90 ± 0.70	kJ/mol	NIST Webbook
hsub	69.90 ± 0.40	kJ/mol	NIST Webbook
hvap	36.86	kJ/mol	Joback Method
ie	8.33	eV	NIST Webbook
ie	8.33	eV	NIST Webbook
ie	8.54	eV	NIST Webbook
log10ws	-1.65		Crippen Method
logp	1.814		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
rinpol	1031.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1027.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1296.00		NIST Webbook
tb	410.80	K	Joback Method
tc	657.97	K	Joback Method
tf	327.20 ± 0.20	K	NIST Webbook
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.39	J/mol×K	451.99	Joback Method
cpg	207.62	J/mol×K	657.97	Joback Method
cpg	199.20	J/mol×K	616.77	Joback Method
cpg	190.10	J/mol×K	575.58	Joback Method
cpg	180.29	J/mol×K	534.38	Joback Method
cpg	169.74	J/mol×K	493.19	Joback Method
cpg	146.23	J/mol×K	410.80	Joback Method
cps	113.90	J/mol×K	300.00	NIST Webbook
hfust	14.40	kJ/mol	327.20	NIST Webbook
hfust	0.80	kJ/mol	316.40	NIST Webbook
hfust	14.40	kJ/mol	327.20	NIST Webbook
hsubt	72.60	kJ/mol	260.50	NIST Webbook
sfust	44.01	J/mol×K	327.20	NIST Webbook
sfust	2.53	J/mol×K	316.40	NIST Webbook

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=C505237&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
cps: Solid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume