1,2-Dithiane

Other names: o-Dithiane
Tetramethylene disulfide
1,2-Dithiacyclohexane
Inchi: InChI=1S/C4H8S2/c1-2-4-6-5-3-1/h1-4H2
InchiKey: CXWGKAYMVASWDQ-UHFFFAOYSA-N
Formula: C4H8S2
SMILES: C1CCSSC1
Mol. weight [g/mol]: 120.24
CAS: 505-20-4

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
hvap	36.86	kJ/mol	Joback Method
ie	8.36	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
log10ws	-2.15		Crippen Method
logp	2.162		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1086.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1489.00		NIST Webbook
tb	410.80	K	Joback Method
tc	657.97	K	Joback Method
tf	313.36	K	Joback Method
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.23	J/mol×K	410.80	Joback Method
cpg	158.39	J/mol×K	451.99	Joback Method
cpg	169.74	J/mol×K	493.19	Joback Method
cpg	180.29	J/mol×K	534.38	Joback Method
cpg	190.10	J/mol×K	575.58	Joback Method
cpg	199.20	J/mol×K	616.77	Joback Method
cpg	207.62	J/mol×K	657.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.20	K	0.70	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=C505204&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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume