1,4-Dithiane

Other names:	1,4-Dithiacyclohexane
	1,4-Dithiin, tetrahydro-
	1,4-dithian
	p-Dithiane
	p-Dithiin, tetrahydro-
	para-Dithiane
Inchi:	InChI=1S/C4H8S2/c1-2-6-4-3-5-1/h1-4H2
InchiKey:	LOZWAPSEEHRYPG-UHFFFAOYSA-N
Formula:	C4H8S2
SMILES:	C1CSCCS1
Mol. weight [g/mol]:	120.24
CAS:	505-29-3

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	63.00	kJ/mol	NIST Webbook
hsub	68.90	kJ/mol	NIST Webbook
hvap	36.86	kJ/mol	Joback Method
ie	8.46	eV	NIST Webbook
ie	8.58	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.80 ± 0.10	eV	NIST Webbook
log10ws	-1.16		Crippen Method
logp	1.466		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
rinpol	1019.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1067.70		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1060.20		NIST Webbook
rinpol	1018.70		NIST Webbook
rinpol	1060.20		NIST Webbook
rinpol	1074.00		NIST Webbook

rinpol	1068.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1060.20		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1022.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1618.90		NIST Webbook
ripol	1575.70		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1575.70		NIST Webbook
tb	472.70	K	NIST Webbook
tc	657.97	K	Joback Method
tf	384.60 ± 0.20	K	NIST Webbook
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	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	146.23	J/mol×K	410.80	Joback Method
cps	129.80	J/mol×K	300.00	NIST Webbook
hfust	21.60	kJ/mol	384.60	NIST Webbook
hfust	21.60	kJ/mol	384.60	NIST Webbook
hfust	21.60	kJ/mol	384.60	NIST Webbook
hsubt	72.40	kJ/mol	264.50	NIST Webbook
hvapt	47.90	kJ/mol	412.50	NIST Webbook
hvapt	48.70	kJ/mol	413.00	NIST Webbook

psub	4.63	kPa	376.95	Vapor Pressure of Solid 1,4-Dithiane
psub	3.91	kPa	374.25	Vapor Pressure of Solid 1,4-Dithiane
psub	2.65	kPa	367.35	Vapor Pressure of Solid 1,4-Dithiane
psub	1.89	kPa	362.35	Vapor Pressure of Solid 1,4-Dithiane
psub	1.33	kPa	359.45	Vapor Pressure of Solid 1,4-Dithiane
psub	1.07	kPa	355.75	Vapor Pressure of Solid 1,4-Dithiane
psub	3.83	kPa	374.05	Vapor Pressure of Solid 1,4-Dithiane
psub	3.25	kPa	370.65	Vapor Pressure of Solid 1,4-Dithiane
sfust	56.20	J/mol×K	384.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.01308e+01
Coeff. B	-1.50998e+03
Coeff. C	-1.98778e+02
Temperature range (K), min.	352.18
Temperature range (K), max.	512.10

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Vapor Pressure of Solid 1,4-Dithiane: https://www.doi.org/10.1021/je800586u

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=C505293&Units=SI

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor 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