

1,2-Dithiolane

Other names:	1,2-Dithiacyclopentane
Inchi:	InChI=1S/C3H6S2/c1-2-4-5-3-1/h1-3H2
InchiKey:	MUZIZEZCKKMZRT-UHFFFAOYSA-N
Formula:	C3H6S2
SMILES:	C1CSSC1
Mol. weight [g/mol]:	106.21
CAS:	557-22-2

Physical Properties

Property code	Value	Unit	Source
gf	98.36	kJ/mol	Joback Method
hf	66.09	kJ/mol	Joback Method
hfus	3.70	kJ/mol	Joback Method
hvap	34.46	kJ/mol	Joback Method
ie	8.25	eV	NIST Webbook
ie	7.60	eV	NIST Webbook
log10ws	-1.73		Crippen Method
logp	1.772		Crippen Method
mcvol	74.970	ml/mol	McGowan Method
pc	5871.90	kPa	Joback Method
rinpol	986.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	963.00		NIST Webbook
ripol	1523.00		NIST Webbook
tb	383.65	K	Joback Method
tc	623.34	K	Joback Method
tf	305.61	K	Joback Method
vc	0.237	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	113.20	J/mol×K	383.65	Joback Method
cpg	122.76	J/mol×K	423.60	Joback Method
cpg	131.61	J/mol×K	463.55	Joback Method
cpg	139.81	J/mol×K	503.50	Joback Method
cpg	147.38	J/mol×K	543.44	Joback Method
cpg	154.38	J/mol×K	583.39	Joback Method
cpg	160.85	J/mol×K	623.34	Joback Method

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=C557222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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