

1,3-Dithiolane-2-thione

Other names:	Carbonic acid, trithio-, cyclic ethylene ester Cyclic ethylene trithiocarbonate Ethylene trithiocarbonate Trithiocarbonic acid, cyclic ethylene ester 1,3-Dithiolan-2-thione 1,3-Dithiacyclopentane-2-thione Cyclic ethylene trithiocarbonate
Inchi:	InChI=1S/C3H4S3/c4-3-5-1-2-6-3/h1-2H2
InchiKey:	XCWPBWWTGHQKDR-UHFFFAOYSA-N
Formula:	C3H4S3
SMILES:	S=C1SCCS1
Mol. weight [g/mol]:	136.26
CAS:	822-38-8

Physical Properties

Property code	Value	Unit	Source
chg	-3571.00 ± 2.00	kJ/mol	NIST Webbook
gf	189.21	kJ/mol	Joback Method
hf	93.80 ± 2.00	kJ/mol	NIST Webbook
hfus	9.74	kJ/mol	Joback Method
hsub	81.80 ± 0.80	kJ/mol	NIST Webbook
hvap	82.90	kJ/mol	NIST Webbook
hvap	81.80 ± 0.80	kJ/mol	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-2.09		Crippen Method
logp	1.751		Crippen Method
mcvol	87.020	ml/mol	McGowan Method
pc	6493.16	kPa	Joback Method
tb	456.29	K	Joback Method
tc	724.56	K	Joback Method
tf	369.28	K	Joback Method
vc	0.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.99	J/mol×K	456.29	Joback Method
cpg	145.47	J/mol×K	501.00	Joback Method
cpg	152.15	J/mol×K	545.71	Joback Method
cpg	158.12	J/mol×K	590.42	Joback Method
cpg	163.46	J/mol×K	635.13	Joback Method
cpg	168.27	J/mol×K	679.85	Joback Method
cpg	172.63	J/mol×K	724.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C822388&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

chg:	Standard gas enthalpy of combustion
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
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/40-291-4/1-3-Dithiolane-2-thione.pdf>

Generated by Cheméo on 2025-12-05 07:56:44.495867667 +0000 UTC m=+4669602.025908332.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.