

1,3-Dithiole, 2-(1,3-dithiol-2-ylidene)-

Other names:	1,4,5,8-Tetrathiafulvalene Tetrathiafulvalene «DELTA»2,2'-Bi-1,3-dithiole «delta»-2:2'-bis(1,3-dithiazole)
Inchi:	InChI=1S/C6H4S4/c1-2-8-5(7-1)6-9-3-4-10-6/h1-4H
InchiKey:	FHCPAXDKURNIOZ-UHFFFAOYSA-N
Formula:	C6H4S4
SMILES:	C1=CSC(=C2SC=CS2)S1
Mol. weight [g/mol]:	204.37
CAS:	31366-25-3

Physical Properties

Property code	Value	Unit	Source
chs	-5619.50 ± 1.70	kJ/mol	NIST Webbook
hfs	290.80 ± 1.70	kJ/mol	NIST Webbook
hfus	14.54	kJ/mol	Joback Method
ie	6.30	eV	NIST Webbook
ie	7.00	eV	NIST Webbook
ie	6.72	eV	NIST Webbook
ie	6.83	eV	NIST Webbook
ie	6.92 ± 0.03	eV	NIST Webbook
ie	6.83	eV	NIST Webbook
logp	4.015		Crippen Method
mcvol	126.180	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.96	J/mol×K	575.34	Joback Method
cpg	241.66	J/mol×K	627.93	Joback Method
cpg	250.21	J/mol×K	680.51	Joback Method
cpg	257.80	J/mol×K	733.10	Joback Method
cpg	264.59	J/mol×K	785.69	Joback Method
cpg	270.74	J/mol×K	838.27	Joback Method

cpg	276.43	J/mol×K	890.86	Joback Method
hsubt	95.00 ± 1.00	kJ/mol	345.00	NIST Webbook
hsubt	92.00 ± 6.30	kJ/mol	351.00	NIST Webbook
hvapt	95.30	kJ/mol	343.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.10780e+01
Coeff. B	-9.44085e+03
Coeff. C	-2.45000e+00
Temperature range (K), min.	456.55
Temperature range (K), max.	601.24

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31366253&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure

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