

1,2,4,5-Tetrathiane

Other names:	s-Tetrathiane 1,2,4,5-Tetrathiacyclohexane
Inchi:	InChI=1S/C2H4S4/c1-3-5-2-6-4-1/h1-2H2
InchiKey:	VXTWQLLUXWBOGW-UHFFFAOYSA-N
Formula:	C2H4S4
SMILES:	C1SSCSS1
Mol. weight [g/mol]:	156.31
CAS:	291-22-5

Physical Properties

Property code	Value	Unit	Source
gf	157.56	kJ/mol	Joback Method
hf	171.09	kJ/mol	Joback Method
hfus	6.33	kJ/mol	Joback Method
hvap	44.03	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.678		Crippen Method
mcvol	93.580	ml/mol	McGowan Method
pc	6990.97	kPa	Joback Method
rinpol	1318.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1337.00		NIST Webbook
tb	460.70	K	Joback Method
tc	755.40	K	Joback Method
tf	457.72	K	Joback Method
vc	0.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.61	J/mol×K	460.70	Joback Method
cpg	155.11	J/mol×K	509.82	Joback Method

cpg	162.82	J/mol×K	558.93	Joback Method
cpg	169.79	J/mol×K	608.05	Joback Method
cpg	176.08	J/mol×K	657.17	Joback Method
cpg	181.76	J/mol×K	706.29	Joback Method
cpg	186.88	J/mol×K	755.40	Joback Method

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=C291225&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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