

4,6-Diethyl-1,2,3,5-tetrathiolane

Other names:	1,2,3,5-Tetrathiane, 4,6-diethyl 4,6-diethyl-1,2,3,5-tetrathiane
Inchi:	InChI=1S/C6H12S4/c1-3-5-7-6(4-2)9-10-8-5/h5-6H,3-4H2,1-2H3
InchiKey:	SBTJQRLWVYRND-UHFFFAOYSA-N
Formula:	C6H12S4
SMILES:	CCC1SSSC(CC)S1
Mol. weight [g/mol]:	212.42

Physical Properties

Property code	Value	Unit	Source
gf	175.82	kJ/mol	Joback Method
hf	47.85	kJ/mol	Joback Method
hfus	18.83	kJ/mol	Joback Method
hvap	52.32	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.235		Crippen Method
mcvol	149.940	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
rinpol	1572.00		NIST Webbook
rinpol	1591.00		NIST Webbook
tb	542.88	K	Joback Method
tc	811.52	K	Joback Method
tf	494.32	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.29	J/molxK	542.88	Joback Method
cpg	328.74	J/molxK	587.65	Joback Method
cpg	343.12	J/molxK	632.43	Joback Method
cpg	356.47	J/molxK	677.20	Joback Method
cpg	368.82	J/molxK	721.97	Joback Method
cpg	380.23	J/molxK	766.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322311&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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