

4-ethyl-6-methyl-1,2,3,5-tetrathiane

Other names:	1,2,3,5-Tetrathiane, 4-ethyl-6-methyl
Inchi:	InChI=1S/C5H10S4/c1-3-5-6-4(2)7-9-8-5/h4-5H,3H2,1-2H3
InchiKey:	VYTCEIIUKULUNE-UHFFFAOYSA-N
Formula:	C5H10S4
SMILES:	CCC1SSSC(C)S1
Mol. weight [g/mol]:	198.39

Physical Properties

Property code	Value	Unit	Source
gf	167.40	kJ/mol	Joback Method
hf	68.49	kJ/mol	Joback Method
hfus	16.24	kJ/mol	Joback Method
hvap	50.09	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.845		Crippen Method
mcvol	135.850	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	1560.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1560.00		NIST Webbook
tb	520.00	K	Joback Method
tc	795.02	K	Joback Method
tf	483.05	K	Joback Method
vc	0.431	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	269.51	J/mol×K	520.00	Joback Method
cpg	283.76	J/mol×K	565.84	Joback Method
cpg	297.01	J/mol×K	611.67	Joback Method
cpg	309.30	J/mol×K	657.51	Joback Method
cpg	320.66	J/mol×K	703.34	Joback Method
cpg	331.13	J/mol×K	749.18	Joback Method
cpg	340.75	J/mol×K	795.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R82099&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

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
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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