

6-methyl-1,2,3,4,5-pentathiane

Inchi:	InChI=1S/C2H4S5/c1-2-3-5-7-6-4-2/h2H,1H3
InchiKey:	WRSINPAGMZEMOU-UHFFFAOYSA-N
Formula:	C2H4S5
SMILES:	CC1SSSSS1
Mol. weight [g/mol]:	188.38

Physical Properties

Property code	Value	Unit	Source
gf	189.71	kJ/mol	Joback Method
hf	196.01	kJ/mol	Joback Method
hfus	11.06	kJ/mol	Joback Method
hvap	49.53	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.672		Crippen Method
mcvol	109.930	ml/mol	McGowan Method
pc	6556.41	kPa	Joback Method
rinpol	1397.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1397.00		NIST Webbook
tb	503.86	K	Joback Method
tc	816.28	K	Joback Method
tf	536.93	K	Joback Method
vc	0.310	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.64	J/mol×K	503.86	Joback Method
cpg	191.43	J/mol×K	555.93	Joback Method
cpg	199.41	J/mol×K	608.00	Joback Method
cpg	206.63	J/mol×K	660.07	Joback Method
cpg	213.16	J/mol×K	712.14	Joback Method
cpg	219.05	J/mol×K	764.21	Joback Method
cpg	224.36	J/mol×K	816.28	Joback Method

Sources

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=R219973&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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