1,2,3,5,6-Pentathiepane, 4,7-dimethyl, #1

Inchi: InChI=1S/C4H8S5/c1-3-5-6-4(2)8-9-7-3/h3-4H,1-2H3/t3-,4-/m1/s1
InchiKey: NGHSPVUOJNZCHU-QWWZWVQMSA-N
Formula: C4H8S5
SMILES: CC1SSSC(C)SS1
Mol. weight [g/mol]: 216.43

Physical Properties

Property code	Value	Unit	Source
gf	186.74	kJ/mol	Joback Method
hf	128.23	kJ/mol	Joback Method
hfus	15.21	kJ/mol	Joback Method
hvap	53.85	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.103		Crippen Method
mcvol	138.110	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method
rinpol	1626.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1626.00		NIST Webbook
tb	549.22	K	Joback Method
tc	858.06	K	Joback Method
tf	551.71	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.08	J/mol×K	549.22	Joback Method
cpg	279.83	J/mol×K	600.69	Joback Method
cpg	292.47	J/mol×K	652.17	Joback Method
cpg	304.03	J/mol×K	703.64	Joback Method
cpg	314.54	J/mol×K	755.11	Joback Method
cpg	324.01	J/mol×K	806.59	Joback Method
cpg	332.48	J/mol×K	858.06	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=R44558&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume