5-ethyl-7-pentyl-1,2,3,4,6-pentathiepane

Other names: 1,2,3,4,6-Pentathiepane, 7-ethyl-5-pentyl
Inchi: InChI=1S/C9H18S5/c1-3-5-6-7-9-10-8(4-2)11-13-14-12-9/h8-9H,3-7H2,1-2H3
InchiKey: UYOUHTYDMFGWKP-UHFFFAOYSA-N
Formula: C9H18S5
SMILES: CCCCCC1SSSSC(CC)S1
Mol. weight [g/mol]: 286.56

Physical Properties

Property code	Value	Unit	Source
gf	228.84	kJ/mol	Joback Method
hf	25.03	kJ/mol	Joback Method
hfus	28.16	kJ/mol	Joback Method
hvap	64.98	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.053		Crippen Method
mcvol	208.560	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	1923.00		NIST Webbook
rinpol	2005.00		NIST Webbook
tb	663.62	K	Joback Method
tc	933.89	K	Joback Method
tf	608.06	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.41	J/mol×K	663.62	Joback Method
cpg	521.75	J/mol×K	708.67	Joback Method
cpg	538.69	J/mol×K	753.71	Joback Method
cpg	554.28	J/mol×K	798.76	Joback Method
cpg	568.58	J/mol×K	843.80	Joback Method
cpg	581.63	J/mol×K	888.85	Joback Method
cpg	593.48	J/mol×K	933.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56713&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
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