2,3,5,6,7-Pentathiaoctane, 4-ethyl

Other names: 4-ethyl-2,3,5,6,7-pentathiaoctane
Inchi: InChI=1S/C5H12S5/c1-4-5(8-6-2)9-10-7-3/h5H,4H2,1-3H3
InchiKey: WQGRDWGJZXYXLX-UHFFFAOYSA-N
Formula: C5H12S5
SMILES: CCC(SSC)SSSC
Mol. weight [g/mol]: 232.47

Physical Properties

Property code	Value	Unit	Source
gf	154.38	kJ/mol	Joback Method
hf	57.54	kJ/mol	Joback Method
hfus	25.83	kJ/mol	Joback Method
hvap	60.42	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.393		Crippen Method
mcvol	163.060	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	1679.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1679.00		NIST Webbook
tb	657.26	K	Joback Method
tc	942.30	K	Joback Method
tf	303.11	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.46	J/mol×K	657.26	Joback Method
cpg	359.93	J/mol×K	704.77	Joback Method
cpg	371.31	J/mol×K	752.27	Joback Method
cpg	381.55	J/mol×K	799.78	Joback Method
cpg	390.58	J/mol×K	847.29	Joback Method
cpg	398.35	J/mol×K	894.79	Joback Method

cpg	404.80	J/mol×K	942.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56795&Units=SI

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