4-Ethyl-2,3,5,6-tetrathiaheptane

Inchi: InChI=1S/C5H12S4/c1-4-5(8-6-2)9-7-3/h5H,4H2,1-3H3
InchiKey: MKQUWWSLZSWEPT-UHFFFAOYSA-N
Formula: C5H12S4
SMILES: CCC(SSC)SSC
Mol. weight [g/mol]: 200.41
CAS: 126876-42-4

Physical Properties

Property code	Value	Unit	Source
gf	121.26	kJ/mol	Joback Method
hf	15.67	kJ/mol	Joback Method
hfus	21.70	kJ/mol	Joback Method
hvap	53.60	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.745		Crippen Method
mcvol	146.710	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	1483.40		NIST Webbook
rinpol	1483.40		NIST Webbook
tb	588.48	K	Joback Method
tc	853.93	K	Joback Method
tf	268.71	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.99	J/mol×K	588.48	Joback Method
cpg	315.45	J/mol×K	632.72	Joback Method
cpg	327.09	J/mol×K	676.96	Joback Method
cpg	337.88	J/mol×K	721.21	Joback Method
cpg	347.78	J/mol×K	765.45	Joback Method
cpg	356.77	J/mol×K	809.69	Joback Method
cpg	364.80	J/mol×K	853.93	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=C126876424&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

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