2,3,5,6-Tetrathiaheptane, 4-ethyl

Inchi: InChI=1S/C5H10S4/c1-2-5-8-6-3-4-7-9-5/h5H,2-4H2,1H3
InchiKey: NUTMZWWGGCPEQF-UHFFFAOYSA-N
Formula: C5H10S4
SMILES: CCC1SSCCSS1
Mol. weight [g/mol]: 198.39

Physical Properties

Property code	Value	Unit	Source
gf	163.01	kJ/mol	Joback Method
hf	82.67	kJ/mol	Joback Method
hfus	13.07	kJ/mol	Joback Method
hvap	50.57	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.499		Crippen Method
mcvol	135.850	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
rinpol	1462.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1452.00		NIST Webbook
tb	528.94	K	Joback Method
tc	815.07	K	Joback Method
tf	483.77	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.47	J/mol×K	528.94	Joback Method
cpg	282.32	J/mol×K	576.63	Joback Method
cpg	296.05	J/mol×K	624.32	Joback Method
cpg	308.70	J/mol×K	672.00	Joback Method
cpg	320.29	J/mol×K	719.69	Joback Method
cpg	330.88	J/mol×K	767.38	Joback Method
cpg	340.50	J/mol×K	815.07	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=R56688&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