1,2,3,5-Tetrathiane, 6-ethyl-4-pentyl

Other names: 4-ethyl-6-pentyl- 1,2,3,5-tetrathiane
4-Pentyl-6-ethyl-1,2,3,5-tetrathiane
Inchi: InChI=1S/C9H18S4/c1-3-5-6-7-9-10-8(4-2)11-13-12-9/h8-9H,3-7H2,1-2H3
InchiKey: MFMHIILUPVLZHI-UHFFFAOYSA-N
Formula: C9H18S4
SMILES: CCCCCC1SSSC(CC)S1
Mol. weight [g/mol]: 254.50

Physical Properties

Property code	Value	Unit	Source
gf	201.08	kJ/mol	Joback Method
hf	-14.07	kJ/mol	Joback Method
hfus	26.60	kJ/mol	Joback Method
hvap	59.00	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.405		Crippen Method
mcvol	192.210	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1791.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1760.20		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1760.20		NIST Webbook
tb	611.52	K	Joback Method
tc	862.08	K	Joback Method
tf	528.13	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.22	J/mol×K	611.52	Joback Method
cpg	473.22	J/mol×K	653.28	Joback Method

cpg	490.01	J/mol×K	695.04	Joback Method
cpg	505.65	J/mol×K	736.80	Joback Method
cpg	520.18	J/mol×K	778.56	Joback Method
cpg	533.65	J/mol×K	820.32	Joback Method
cpg	546.11	J/mol×K	862.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56674&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

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