6-Ethyl-4,5,7,8-tetrathia-2-nonene

Other names: 2,3,5,6-Tetrathia-7-nonene, 4-ethyl
4,5,7,8-Tetrathio-2-nonene, 6-ethyl
4-ethyl-2,3,5,6-tetrathia-7-nonene
Inchi: InChI=1S/C7H14S4/c1-4-6-9-11-7(5-2)10-8-3/h4,6-7H,5H2,1-3H3/b6-4+
InchiKey: CKHVKHMFOAPYLZ-GQCTYLIASA-N
Formula: C7H14S4
SMILES: CC=CSSC(CC)SSC
Mol. weight [g/mol]: 226.45

Physical Properties

Property code	Value	Unit	Source
gf	218.32	kJ/mol	Joback Method
hf	91.61	kJ/mol	Joback Method
hfus	27.09	kJ/mol	Joback Method
hvap	58.01	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.649		Crippen Method
mcvol	170.590	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	638.40	K	Joback Method
tc	903.08	K	Joback Method
tf	286.17	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.09	J/mol×K	638.40	Joback Method
cpg	388.74	J/mol×K	682.51	Joback Method
cpg	401.36	J/mol×K	726.63	Joback Method
cpg	412.95	J/mol×K	770.74	Joback Method
cpg	423.52	J/mol×K	814.85	Joback Method

cpg	433.06	J/mol×K	858.97	Joback Method
cpg	441.59	J/mol×K	903.08	Joback Method

Sources

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=U322300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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