7-methyl-4,5,6,9-tetrathia-1,11-dodecadiene

Inchi: InChI=1S/C9H16S4/c1-4-6-10-8-9(3)12-13-11-7-5-2/h4-5,9H,1-2,6-8H2,3H3
InchiKey: ZYOACKSTGJDIHX-UHFFFAOYSA-N
Formula: C9H16S4
SMILES: C=CCSCC(C)SSSCC=C
Mol. weight [g/mol]: 252.48

Physical Properties

Property code	Value	Unit	Source
gf	330.62	kJ/mol	Joback Method
hf	183.97	kJ/mol	Joback Method
hfus	29.50	kJ/mol	Joback Method
hvap	61.17	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.510		Crippen Method
mcvol	194.470	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1819.00		NIST Webbook
tb	673.36	K	Joback Method
tc	925.93	K	Joback Method
tf	310.27	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.20	J/mol×K	673.36	Joback Method
cpg	465.49	J/mol×K	715.45	Joback Method
cpg	478.66	J/mol×K	757.55	Joback Method
cpg	490.75	J/mol×K	799.64	Joback Method
cpg	501.74	J/mol×K	841.74	Joback Method
cpg	511.66	J/mol×K	883.83	Joback Method
cpg	520.52	J/mol×K	925.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225824&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