7-methyl-4,5,8-trithia-1,10-undecadiene

Other names: 7-methyl-4,5,8-trithiaundeca-1,10-diene
Inchi: InChI=1S/C9H16S3/c1-4-6-10-9(3)8-12-11-7-5-2/h4-5,9H,1-2,6-8H2,3H3
InchiKey: DGIXPEPNCCYHNK-UHFFFAOYSA-N
Formula: C9H16S3
SMILES: C=CCSSCC(C)SCC=C
Mol. weight [g/mol]: 220.42

Physical Properties

Property code	Value	Unit	Source
gf	297.50	kJ/mol	Joback Method
hf	142.10	kJ/mol	Joback Method
hfus	25.37	kJ/mol	Joback Method
hvap	54.35	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.861		Crippen Method
mcvol	178.120	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1581.00		NIST Webbook
rinpol	1593.00		NIST Webbook
ripol	2202.00		NIST Webbook
ripol	2202.00		NIST Webbook
tb	604.58	K	Joback Method
tc	839.74	K	Joback Method
tf	275.87	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.66	J/mol×K	604.58	Joback Method
cpg	415.21	J/mol×K	643.77	Joback Method
cpg	428.83	J/mol×K	682.97	Joback Method
cpg	441.54	J/mol×K	722.16	Joback Method
cpg	453.35	J/mol×K	761.35	Joback Method

cpg	464.28	J/mol×K	800.55	Joback Method
cpg	474.35	J/mol×K	839.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R222612&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume