6-Methyl-4,5,8-trithia-1,10-undecadiene

Inchi: InChI=1S/C9H16S3/c1-4-6-10-8-9(3)12-11-7-5-2/h4-5,9H,1-2,6-8H2,3H3
InchiKey: NZIHHTYFEJSFCC-UHFFFAOYSA-N
Formula: C9H16S3
SMILES: C=CCSCC(C)SSCC=C
Mol. weight [g/mol]: 220.42
CAS: 116664-22-3

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	1591.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1602.70		NIST Webbook
rinpol	1602.70		NIST Webbook
ripol	2213.00		NIST Webbook
ripol	2213.00		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=C116664223&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