8-methyl-4,5,6,7,10-pentathia-1,12-tridecadiene

Inchi: InChI=1S/C9H16S5/c1-4-6-10-8-9(3)12-14-13-11-7-5-2/h4-5,9H,1-2,6-8H2,3H3
InchiKey: NGDHBSGNCAGFLV-UHFFFAOYSA-N
Formula: C9H16S5
SMILES: C=CCSCC(C)SSSSCC=C
Mol. weight [g/mol]: 284.55

Physical Properties

Property code	Value	Unit	Source
gf	363.74	kJ/mol	Joback Method
hf	225.84	kJ/mol	Joback Method
hfus	33.63	kJ/mol	Joback Method
hvap	67.99	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.158		Crippen Method
mcvol	210.820	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	2061.00		NIST Webbook
rinpol	2061.00		NIST Webbook
tb	742.14	K	Joback Method
tc	1010.80	K	Joback Method
tf	344.67	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.26	J/mol×K	742.14	Joback Method
cpg	513.84	J/mol×K	786.92	Joback Method
cpg	526.08	J/mol×K	831.69	Joback Method
cpg	536.99	J/mol×K	876.47	Joback Method
cpg	546.55	J/mol×K	921.25	Joback Method
cpg	554.78	J/mol×K	966.03	Joback Method
cpg	561.65	J/mol×K	1010.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225839&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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