4-methyl-3-thia-1-pentene

Other names: Propane, 2-ethenylthio-
Inchi: InChI=1S/C5H10S/c1-4-6-5(2)3/h4-5H,1H2,2-3H3
InchiKey: KENPNZJNGZPRCQ-UHFFFAOYSA-N
Formula: C5H10S
SMILES: C=CSC(C)C
Mol. weight [g/mol]: 102.20
CAS: 18888-46-5

Physical Properties

Property code	Value	Unit	Source
gf	109.74	kJ/mol	Joback Method
hf	15.49	kJ/mol	Joback Method
hfus	8.03	kJ/mol	Joback Method
hvap	32.48	kJ/mol	Joback Method
ie	8.15 ± 0.01	eV	NIST Webbook
log10ws	-2.26		Crippen Method
logp	2.272		Crippen Method
mcvol	93.360	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
rinpol	740.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	740.00		NIST Webbook
tb	378.82	K	Joback Method
tc	578.03	K	Joback Method
tf	163.75	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.65	J/mol×K	378.82	Joback Method
cpg	165.33	J/mol×K	412.02	Joback Method
cpg	174.60	J/mol×K	445.22	Joback Method
cpg	183.46	J/mol×K	478.43	Joback Method

cpg	191.93	J/mol×K	511.63	Joback Method
cpg	200.01	J/mol×K	544.83	Joback Method
cpg	207.71	J/mol×K	578.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18888465&Units=SI

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
ie:	Ionization energy
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