4-methyl-3-thia-1-hexene

Other names: Butane, 2-ethenylthio
Inchi: InChI=1S/C6H12S/c1-4-6(3)7-5-2/h5-6H,2,4H2,1,3H3
InchiKey: XJFDZBUNGBVGEV-UHFFFAOYSA-N
Formula: C6H12S
SMILES: C=CSC(C)CC
Mol. weight [g/mol]: 116.22

Physical Properties

Property code	Value	Unit	Source
gf	118.16	kJ/mol	Joback Method
hf	-5.15	kJ/mol	Joback Method
hfus	10.62	kJ/mol	Joback Method
hvap	34.71	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.662		Crippen Method
mcvol	107.450	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	845.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	845.00		NIST Webbook
tb	401.70	K	Joback Method
tc	599.38	K	Joback Method
tf	175.02	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.61	J/mol×K	401.70	Joback Method
cpg	202.77	J/mol×K	434.65	Joback Method
cpg	213.45	J/mol×K	467.59	Joback Method
cpg	223.65	J/mol×K	500.54	Joback Method
cpg	233.39	J/mol×K	533.49	Joback Method
cpg	242.67	J/mol×K	566.43	Joback Method

cpg	251.51	J/mol×K	599.38	Joback Method

Sources

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=R144002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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