5,6-dimethyl-4-thia-1-heptene

Other names: Allyl (1,2-dimethylpropyl) sulfide
Inchi: InChI=1S/C8H16S/c1-5-6-9-8(4)7(2)3/h5,7-8H,1,6H2,2-4H3
InchiKey: AVHRBMFFYICAIH-UHFFFAOYSA-N
Formula: C8H16S
SMILES: C=CCSC(C)C(C)C
Mol. weight [g/mol]: 144.28

Physical Properties

Property code	Value	Unit	Source
gf	132.56	kJ/mol	Joback Method
hf	-51.71	kJ/mol	Joback Method
hfus	12.28	kJ/mol	Joback Method
hvap	38.77	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.950		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	997.00		NIST Webbook
rinpol	997.00		NIST Webbook
tb	447.02	K	Joback Method
tc	645.40	K	Joback Method
tf	182.56	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.62	J/mol×K	447.02	Joback Method
cpg	284.70	J/mol×K	480.08	Joback Method
cpg	298.12	J/mol×K	513.15	Joback Method
cpg	310.92	J/mol×K	546.21	Joback Method
cpg	323.11	J/mol×K	579.28	Joback Method
cpg	334.69	J/mol×K	612.34	Joback Method
cpg	345.69	J/mol×K	645.40	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=R144037&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