5-methyl-4-thia-1-heptene

Other names: Sulfide, allyl sec-butyl,
Inchi: InChI=1S/C7H14S/c1-4-6-8-7(3)5-2/h4,7H,1,5-6H2,2-3H3
InchiKey: QLCUOCVKHIAUIL-UHFFFAOYSA-N
Formula: C7H14S
SMILES: C=CCSC(C)CC
Mol. weight [g/mol]: 130.25
CAS: 70289-07-5

Physical Properties

Property code	Value	Unit	Source
gf	126.58	kJ/mol	Joback Method
hf	-25.79	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.704		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook
tb	424.58	K	Joback Method
tc	620.45	K	Joback Method
tf	186.29	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.95	J/mol×K	424.58	Joback Method
cpg	242.43	J/mol×K	457.22	Joback Method
cpg	254.37	J/mol×K	489.87	Joback Method
cpg	265.77	J/mol×K	522.51	Joback Method
cpg	276.65	J/mol×K	555.16	Joback Method
cpg	287.01	J/mol×K	587.80	Joback Method

cpg	296.87	J/mol×K	620.45	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=C70289075&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
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