3-((1,1-Dimethylethyl)-thio)-1-propene

Other names: Allyl tert-butyl sulphide
Allyl sec-butyl sulfide
5,5-Dimethyl-4-thia-1-hexene
Inchi: InChI=1S/C7H14S/c1-5-6-8-7(2,3)4/h5H,1,6H2,2-4H3
InchiKey: XIBMCVKDUXKQRS-UHFFFAOYSA-N
Formula: C7H14S
SMILES: C=CCSC(C)(C)C
Mol. weight [g/mol]: 130.25
CAS: 37850-75-2

Physical Properties

Property code	Value	Unit	Source
chl	-5266.60 ± 2.50	kJ/mol	NIST Webbook
gf	131.86	kJ/mol	Joback Method
hf	-46.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-90.70 ± 1.60	kJ/mol	NIST Webbook
hfus	9.32	kJ/mol	Joback Method
hvap	44.70	kJ/mol	NIST Webbook
hvap	44.80	kJ/mol	NIST Webbook
hvap	44.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-2.60		Crippen Method
logp	2.704		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	855.70		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	877.00		NIST Webbook
tb	421.79	K	Joback Method
tc	626.22	K	Joback Method
tf	203.71	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.80	J/mol×K	558.08	Joback Method
cpg	292.48	J/mol×K	592.15	Joback Method
cpg	232.08	J/mol×K	421.79	Joback Method
cpg	245.62	J/mol×K	455.86	Joback Method
cpg	258.40	J/mol×K	489.93	Joback Method
cpg	270.45	J/mol×K	524.01	Joback Method
cpg	302.53	J/mol×K	626.22	Joback Method
hvapt	41.90	kJ/mol	329.00	NIST Webbook
hvapt	43.10	kJ/mol	329.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37850752&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

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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