

Allyl(ethyl)sulfide

Other names:	4-Thia-1-hexene Allyl ethyl sulfide Allyl ethyl sulphide <chem>CH2=CHCH2SC2H5</chem>
Inchi:	InChI=1S/C5H10S/c1-3-5-6-4-2/h3H,1,4-5H2,2H3
InchiKey:	NOJXPGXFDASWEI-UHFFFAOYSA-N
Formula:	C5H10S
SMILES:	<chem>C=CCSCC</chem>
Mol. weight [g/mol]:	102.20
CAS:	5296-62-8

Physical Properties

Property code	Value	Unit	Source
af	0.1816		Cheméo Relay (1.0)
chl	-3977.40 ± 1.90	kJ/mol	NIST Webbook
gf	112.18	kJ/mol	Joback Method
hf	18.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-21.00 ± 3.00	kJ/mol	NIST Webbook
hfus	11.56	kJ/mol	Joback Method
hvap	39.00	kJ/mol	NIST Webbook
hvap	39.30	kJ/mol	NIST Webbook
hvap	39.00 ± 1.00	kJ/mol	NIST Webbook
ie	8.51 ± 0.01	eV	NIST Webbook
log10ws	-1.69		Cheméo Relay (1.0)
logp	1.925		Crippen Method
mcvol	93.360	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	777.00		NIST Webbook
rinpol	777.00		NIST Webbook
tb	389.60	K	Cheméo Relay (1.0)
tc	568.76	K	Cheméo Relay (1.0)
tf	146.71	K	Cheméo Relay (1.0)
vc	0.321	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.70	J/mol×K	379.26	Joback Method
cpg	165.05	J/mol×K	411.65	Joback Method
cpg	174.01	J/mol×K	444.04	Joback Method
cpg	182.59	J/mol×K	476.44	Joback Method
cpg	190.80	J/mol×K	508.83	Joback Method
cpg	198.64	J/mol×K	541.22	Joback Method
cpg	206.14	J/mol×K	573.61	Joback Method
hvapt	38.90	kJ/mol	313.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	7.01322e+00
Coeff. B	-5.54504e+02
Coeff. C	-2.05297e+02
Temperature range (K), min.	287.74
Temperature range (K), max.	531.14

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5296628&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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