

Propane, 1-(ethenylthio)-

Other names:	1-(Propylsulfanyl)ethylene 3-Thia-1-hexene
Inchi:	InChI=1S/C5H10S/c1-3-5-6-4-2/h4H,2-3,5H2,1H3
InchiKey:	HWRMMWBUMQCMJK-UHFFFAOYSA-N
Formula:	C5H10S
SMILES:	C=CSCCC
Mol. weight [g/mol]:	102.20
CAS:	16330-21-5

Physical Properties

Property code	Value	Unit	Source
gf	112.18	kJ/mol	Joback Method
hf	20.77	kJ/mol	Joback Method
hfus	11.56	kJ/mol	Joback Method
hvap	32.87	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.273		Crippen Method
mvol	93.360	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinp	794.00		NIST Webbook
tb	379.26	K	Joback Method
tc	573.61	K	Joback Method
tf	178.75	K	Joback Method
vc	0.350	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.70	J/molxK	379.26	Joback Method
cpg	165.05	J/molxK	411.65	Joback Method
cpg	174.01	J/molxK	444.04	Joback Method
cpg	182.59	J/molxK	476.44	Joback Method
cpg	190.80	J/molxK	508.83	Joback Method
cpg	198.64	J/molxK	541.22	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=C16330215&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

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