

1-propenyl hydrodisulfide

Inchi:	InChI=1S/C3H6S2/c1-2-3-5-4/h2-4H,1H3/b3-2+
InchiKey:	OMMJRBQXFJVFFD-NSCUHMNNSA-N
Formula:	C3H6S2
SMILES:	CC=CSS
Mol. weight [g/mol]:	106.21

Physical Properties

Property code	Value	Unit	Source
gf	117.11	kJ/mol	Joback Method
hf	92.32	kJ/mol	Joback Method
hfus	11.90	kJ/mol	Joback Method
hvap	35.78	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.098		Crippen Method
mcvol	81.530	ml/mol	McGowan Method
pc	5304.68	kPa	Joback Method
rinpol	835.00		NIST Webbook
rinpol	845.00		NIST Webbook
tb	403.84	K	Joback Method
tc	637.01	K	Joback Method
tf	189.35	K	Joback Method
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.73	J/molxK	403.84	Joback Method
cpg	130.86	J/molxK	442.70	Joback Method
cpg	137.57	J/molxK	481.56	Joback Method
cpg	143.88	J/molxK	520.42	Joback Method
cpg	149.80	J/molxK	559.28	Joback Method
cpg	155.35	J/molxK	598.15	Joback Method
cpg	160.56	J/molxK	637.01	Joback Method

Sources

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=R220498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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