

Disulfide, 1-propenyl, 2-propenyl, #1

Other names:	allyl trans-1-propenyl disulfide
Inchi:	InChI=1S/C6H10S2/c1-3-5-7-8-6-4-2/h3-4,6H,1,5H2,2H3/b6-4+
InchiKey:	KBXOGESWPIVMNJ-GQCTYLIASA-N
Formula:	C6H10S2
SMILES:	C=CCSSC=CC
Mol. weight [g/mol]:	146.27

Physical Properties

Property code	Value	Unit	Source
gf	233.94	kJ/mol	Joback Method
hf	159.22	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	41.87	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.087		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	1081.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1074.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1533.00		NIST Webbook
tb	475.08	K	Joback Method
tc	703.14	K	Joback Method
tf	219.34	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.99	J/mol×K	475.08	Joback Method
cpg	230.97	J/mol×K	513.09	Joback Method
cpg	241.30	J/mol×K	551.10	Joback Method
cpg	251.02	J/mol×K	589.11	Joback Method
cpg	260.14	J/mol×K	627.12	Joback Method
cpg	268.70	J/mol×K	665.13	Joback Method
cpg	276.70	J/mol×K	703.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R82227&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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