

1-((E)-Prop-1-en-1-yl)-2-((Z)-prop-1-en-1-yl)disulfane

Inchi:	InChI=1S/C6H10S2/c1-3-5-7-8-6-4-2/h3-6H,1-2H3/b5-3-,6-4+
InchiKey:	FHSDVOJKLYJNCQ-CIIODKQPSA-N
Formula:	C6H10S2
SMILES:	CC=CSSC=CC
Mol. weight [g/mol]:	146.27
CAS:	121609-82-3

Physical Properties

Property code	Value	Unit	Source
gf	226.32	kJ/mol	Joback Method
hf	151.01	kJ/mol	Joback Method
hfus	19.96	kJ/mol	Joback Method
hvap	42.50	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.435		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	1124.00		NIST Webbook
rinpol	1124.00		NIST Webbook
tb	482.56	K	Joback Method
tc	716.77	K	Joback Method
tf	216.02	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.51	J/molxK	482.56	Joback Method
cpg	230.71	J/molxK	521.60	Joback Method
cpg	241.19	J/molxK	560.63	Joback Method
cpg	250.99	J/molxK	599.67	Joback Method
cpg	260.15	J/molxK	638.70	Joback Method
cpg	268.71	J/molxK	677.74	Joback Method
cpg	276.70	J/molxK	716.77	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=C121609823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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