Diallyl sulfide

Other names:	Allyl sulfide
	1-Propene, 3,3'-thiobis-
	Allyl monosulfide
	Diallyl monosulfide
	Diallyl thioether
	Oil garlic
	Thioallyl ether
	(CH2=CHCH2)2S
	2-Propenyl sulphide
	3,3-Thiobis(1-propene)
	Allyl sulphide
	di-2-Propenyl sulfide
	Diallyl sulphide
	Prop-1-ene-3,3'-thiobis
	NSC 20947
Inchi:	InChI=1S/C6H10S/c1-3-5-7-6-4-2/h3-4H,1-2,5-6H2
InchiKey:	UBJVUCKUDDKUJF-UHFFFAOYSA-N
Formula:	C6H10S
SMILES:	C=CCSCC=C
Mol. weight [g/mol]:	114.21
CAS:	592-88-1

Physical Properties

Property code	Value	Unit	Source
chl	-4468.90	kJ/mol	NIST Webbook
gf	208.44	kJ/mol	Joback Method
hf	125.56	kJ/mol	Joback Method
hfus	12.87	kJ/mol	Joback Method
hvap	34.43	kJ/mol	Joback Method
ie	8.52 ± 0.01	eV	NIST Webbook
log10ws	-1.93		Crippen Method
logp	2.092		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
rinpol	850.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	848.00		NIST Webbook

rinpol	848.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	831.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	849.00	NIST Webbook
rinpol	852.00	NIST Webbook
rinpol	852.00	NIST Webbook
rinpol	872.00	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	867.00	NIST Webbook
rinpol	861.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	864.60	NIST Webbook
rinpol	871.60	NIST Webbook
rinpol	856.20	NIST Webbook
rinpol	860.30	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	850.00	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	850.00	NIST Webbook
rinpol	863.00	NIST Webbook
rinpol	850.00	NIST Webbook
rinpol	858.80	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	860.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	871.00	NIST Webbook
ripol	1145.00	NIST Webbook
ripol	1151.00	NIST Webbook
ripol	1142.00	NIST Webbook
ripol	1150.00	NIST Webbook
ripol	1164.00	NIST Webbook
ripol	1118.00	NIST Webbook
ripol	1148.00	NIST Webbook
ripol	1143.00	NIST Webbook
ripol	1150.00	NIST Webbook
ripol	1150.00	NIST Webbook
ripol	1148.00	NIST Webbook
ripol	1148.00	NIST Webbook
ripol	1148.00	NIST Webbook
ripol	1118.00	NIST Webbook

ripol	1149.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1143.00		NIST Webbook
ripol	1147.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1143.00		NIST Webbook
tb	411.20	K	NIST Webbook
tb	411.00	K	NIST Webbook
tb	412.00 ± 3.00	K	NIST Webbook
tc	596.11	K	Joback Method
tf	188.26	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.96	J/mol×K	398.82	Joback Method
cpg	187.06	J/mol×K	431.70	Joback Method
cpg	196.68	J/mol×K	464.58	Joback Method
cpg	205.83	J/mol×K	497.46	Joback Method
cpg	214.54	J/mol×K	530.34	Joback Method
cpg	222.82	J/mol×K	563.22	Joback Method
cpg	230.67	J/mol×K	596.11	Joback Method
hvapt	46.60	kJ/mol	337.00	NIST Webbook
hvapt	43.20	kJ/mol	337.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C592881&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

Legend

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
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
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