propyl allyl disulfide

Other names:	Allyl propyl disulfide
	4,5-dithia-1-octene
	2-propenyl propyl disulfide
	Propyl 2-propenyl disulfide
	Allyl propyl disulphide
Inchi:	InChI=1S/C6H12S2/c1-3-5-7-8-6-4-2/h3H,1,4-6H2,2H3
InchiKey:	FCSSPCOFDUKHPV-UHFFFAOYSA-N
Formula:	C6H12S2
SMILES:	C=CCSSCCC
Mol. weight [g/mol]:	148.29
CAS:	2179-59-1

Physical Properties

Property code	Value	Unit	Source
gf	153.72	kJ/mol	Joback Method
hf	42.00	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	41.91	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.964		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	1048.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1077.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1436.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1436.00		NIST Webbook

ripol	1410.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1432.00		NIST Webbook
tb	470.92	K	Joback Method
tc	687.95	K	Joback Method
tf	224.42	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.15	J/mol×K	470.92	Joback Method
cpg	248.69	J/mol×K	507.09	Joback Method
cpg	259.67	J/mol×K	543.26	Joback Method
cpg	270.11	J/mol×K	579.43	Joback Method
cpg	280.01	J/mol×K	615.61	Joback Method
cpg	289.38	J/mol×K	651.78	Joback Method
cpg	298.22	J/mol×K	687.95	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2179591&Units=SI

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