Disulfide, 1-(1-propenyldithio)propyl propyl, (Z)-

Inchi: InChI=1S/C9H18S4/c1-4-7-10-12-9(6-3)13-11-8-5-2/h4,7,9H,5-6,8H2,1-3H3/b7-4-
InchiKey: MMZWJALGNZCSLI-DAXSKMNVSA-N
Formula: C9H18S4
SMILES: CC=CSSC(CC)SSCCC
Mol. weight [g/mol]: 254.50
CAS: 126876-37-7

Physical Properties

Property code	Value	Unit	Source
gf	235.16	kJ/mol	Joback Method
hf	50.33	kJ/mol	Joback Method
hfus	32.26	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.429		Crippen Method
mcvol	198.770	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1809.60		NIST Webbook
tb	684.16	K	Joback Method
tc	936.50	K	Joback Method
tf	308.71	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.10	J/mol×K	684.16	Joback Method
cpg	489.15	J/mol×K	726.22	Joback Method
cpg	503.06	J/mol×K	768.27	Joback Method
cpg	515.85	J/mol×K	810.33	Joback Method
cpg	527.53	J/mol×K	852.39	Joback Method
cpg	538.11	J/mol×K	894.45	Joback Method
cpg	547.62	J/mol×K	936.50	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=C126876377&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume