(E)-sec-Butyl propenyl disulfide

Inchi: InChI=1S/C7H14S2/c1-4-6-8-9-7(3)5-2/h4,6-7H,5H2,1-3H3/b6-4+
InchiKey: IOVUOUZQSDBAQN-GQCTYLIASA-N
Formula: C7H14S2
SMILES: CC=CSSC(C)CC
Mol. weight [g/mol]: 162.32
CAS: 24351-71-1

Physical Properties

Property code	Value	Unit	Source
gf	152.08	kJ/mol	Joback Method
hf	7.87	kJ/mol	Joback Method
hfus	18.82	kJ/mol	Joback Method
hvap	44.38	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.700		Crippen Method
mcvol	137.890	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1182.10		NIST Webbook
rinpol	1182.10		NIST Webbook
tb	500.84	K	Joback Method
tc	725.26	K	Joback Method
tf	217.37	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.01	J/mol×K	500.84	Joback Method
cpg	292.38	J/mol×K	538.24	Joback Method
cpg	305.02	J/mol×K	575.65	Joback Method
cpg	316.95	J/mol×K	613.05	Joback Method
cpg	328.19	J/mol×K	650.45	Joback Method
cpg	338.77	J/mol×K	687.85	Joback Method
cpg	348.69	J/mol×K	725.26	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=C24351711&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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