Bis(1-methyl propenyl) disulfide

Inchi: InChI=1S/C8H14S2/c1-5-7(3)9-10-8(4)6-2/h5-6H,1-4H3/b7-5+,8-6+
InchiKey: SEUXDSIHTAQGIQ-KQQUZDAGSA-N
Formula: C8H14S2
SMILES: CC=C(C)SSC(C)=CC
Mol. weight [g/mol]: 174.33

Physical Properties

Property code	Value	Unit	Source
gf	226.06	kJ/mol	Joback Method
hf	90.15	kJ/mol	Joback Method
hfus	22.52	kJ/mol	Joback Method
hvap	47.11	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.215		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	1263.00		NIST Webbook
rinpol	1263.00		NIST Webbook
tb	528.08	K	Joback Method
tc	762.98	K	Joback Method
tf	210.64	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.96	J/mol×K	528.08	Joback Method
cpg	317.89	J/mol×K	567.23	Joback Method
cpg	330.94	J/mol×K	606.38	Joback Method
cpg	343.16	J/mol×K	645.53	Joback Method
cpg	354.59	J/mol×K	684.68	Joback Method
cpg	365.27	J/mol×K	723.83	Joback Method
cpg	375.27	J/mol×K	762.98	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=R415879&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