Methyl trans-1-propenyl disulfide

Inchi: InChI=1S/C4H8S2/c1-3-4-6-5-2/h3-4H,1-2H3/b4-3+
InchiKey: FUDUFCLRGSEHAJ-ONEGZZNKSA-N
Formula: C4H8S2
SMILES: CC=CSSC
Mol. weight [g/mol]: 120.24

Physical Properties

Property code	Value	Unit	Source
gf	129.26	kJ/mol	Joback Method
hf	75.07	kJ/mol	Joback Method
hfus	14.58	kJ/mol	Joback Method
hvap	38.09	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.531		Crippen Method
mcvol	95.620	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
rinpol	937.00		NIST Webbook
tb	432.64	K	Joback Method
tc	662.52	K	Joback Method
tf	198.56	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.54	J/mol×K	432.64	Joback Method
cpg	168.42	J/mol×K	470.95	Joback Method
cpg	176.85	J/mol×K	509.27	Joback Method
cpg	184.83	J/mol×K	547.58	Joback Method
cpg	192.36	J/mol×K	585.89	Joback Method
cpg	199.47	J/mol×K	624.20	Joback Method
cpg	206.15	J/mol×K	662.52	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=R612332&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

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