(E)-Methyl-1-propenyl disulfide

Other names: Methyl 1-propenyl disulfide (E)
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
CAS: 23838-19-9

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	940.10		NIST Webbook
rinpol	940.10		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1110.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1332.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23838199&Units=SI
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

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