

Methyl vinyl sulfide

Inchi: InChI=1S/C3H6S/c1-3-4-2/h3H,1H2,2H3
InchiKey: AMBKPYJJYUKNFI-UHFFFAOYSA-N
Formula: C3H6S
SMILES: C=CSC
Mol. weight [g/mol]: 74.14
CAS: 1822-74-8

Physical Properties

Property code	Value	Unit	Source
affp	858.20	kJ/mol	NIST Webbook
basg	829.30	kJ/mol	NIST Webbook
gf	95.34	kJ/mol	Joback Method
hf	62.05	kJ/mol	Joback Method
hfus	6.38	kJ/mol	Joback Method
hvap	28.42	kJ/mol	Joback Method
ie	8.44	eV	NIST Webbook
ie	8.45	eV	NIST Webbook
ie	8.45	eV	NIST Webbook
ie	8.45	eV	NIST Webbook
log10ws	-1.31		Crippen Method
logp	1.493		Crippen Method
mcvol	65.180	ml/mol	McGowan Method
pc	4775.98	kPa	Joback Method
rinpol	608.00		NIST Webbook
rinpol	608.00		NIST Webbook
tb	339.75 ± 0.60	K	NIST Webbook
tb	343.15 ± 2.00	K	NIST Webbook
tb	342.70	K	NIST Webbook
tc	529.43	K	Joback Method
tf	156.21	K	Joback Method
vc	0.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.50	J/mol×K	333.50	Joback Method
cpg	97.48	J/mol×K	366.15	Joback Method
cpg	103.23	J/mol×K	398.81	Joback Method
cpg	108.75	J/mol×K	431.46	Joback Method
cpg	114.06	J/mol×K	464.12	Joback Method
cpg	119.15	J/mol×K	496.77	Joback Method
cpg	124.02	J/mol×K	529.43	Joback Method

Sources

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=C1822748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
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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