

Divinyl sulfoxide

Other names:	Vinyl sulfoxide
Inchi:	InChI=1S/C4H6OS/c1-3-6(5)4-2/h3-4H,1-2H2
InchiKey:	HQSMEHLVLOGBCK-UHFFFAOYSA-N
Formula:	C4H6OS
SMILES:	C=CS(=O)C=C
Mol. weight [g/mol]:	102.16
CAS:	1115-15-7

Physical Properties

Property code	Value	Unit	Source
gf	-59.23	kJ/mol	Joback Method
hf	25.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-26.20 ± 2.50	kJ/mol	NIST Webbook
hfus	11.31	kJ/mol	Joback Method
hvap	51.20 ± 0.90	kJ/mol	NIST Webbook
hvap	51.20 ± 0.90	kJ/mol	NIST Webbook
log10ws	-0.83		Crippen Method
logp	1.022		Crippen Method
mcpvol	80.840	ml/mol	McGowan Method
pc	4876.56	kPa	Joback Method
rinpol	916.00		NIST Webbook
rinpol	916.00		NIST Webbook
tb	342.56	K	Joback Method
tc	526.67	K	Joback Method
tf	167.80	K	Joback Method
vc	0.311	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	121.38	J/mol×K	342.56	Joback Method
cpg	128.57	J/mol×K	373.25	Joback Method
cpg	135.45	J/mol×K	403.93	Joback Method
cpg	142.04	J/mol×K	434.62	Joback Method

cpg	148.35	J/mol×K	465.30	Joback Method
cpg	154.37	J/mol×K	495.99	Joback Method
cpg	160.11	J/mol×K	526.67	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=C1115157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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