

Divinyl sulfide

Other names:	Ethene, 1,1'-thiobis- Vinyl sulfide Divinyl thioether (CH ₂ =CH) ₂ S
Inchi:	InChI=1S/C4H6S/c1-3-5-4-2/h3-4H,1-2H2
InchiKey:	UIYCHXAGWOYNNA-UHFFFAOYSA-N
Formula:	C ₄ H ₆ S
SMILES:	C=CSC=C
Mol. weight [g/mol]:	86.16
CAS:	627-51-0

Physical Properties

Property code	Value	Unit	Source
gf	191.60	kJ/mol	Joback Method
hf	106.00 ± 4.00	kJ/mol	NIST Webbook
hfl	67.70 ± 3.00	kJ/mol	NIST Webbook
hfus	7.69	kJ/mol	Joback Method
hvap	38.30 ± 0.70	kJ/mol	NIST Webbook
hvap	38.30 ± 0.70	kJ/mol	NIST Webbook
hvap	38.30	kJ/mol	NIST Webbook
ie	8.25 ± 0.01	eV	NIST Webbook
ie	8.42	eV	NIST Webbook
log10ws	-2.08		Crippen Method
logp	2.007		Crippen Method
mcpol	74.970	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
rinpol	647.00		NIST Webbook
tb	353.06	K	Joback Method
tc	552.91	K	Joback Method
tf	165.72	K	Joback Method
vc	0.276	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	109.33	J/mol×K	353.06	Joback Method
cpg	116.28	J/mol×K	386.37	Joback Method
cpg	122.90	J/mol×K	419.68	Joback Method
cpg	129.20	J/mol×K	452.98	Joback Method
cpg	135.19	J/mol×K	486.29	Joback Method
cpg	140.87	J/mol×K	519.60	Joback Method
cpg	146.27	J/mol×K	552.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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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