Divinyl sulphone

Other names:	1,1'-Sulphonylbisethene
	(CH2=CH)2SO2
	Divinyl sulfone
	Vinyl sulfone
	Ethene, 1,1'-sulfonylbis-
	Bis(ethenyl)sulfone
	Sulfone, divinyl-
	TL 797
Inchi:	InChI=1S/C4H6O2S/c1-3-7(5,6)4-2/h3-4H,1-2H2
InchiKey:	AFOSIXZFDONLBT-UHFFFAOYSA-N
Formula:	C4H6O2S
SMILES:	C=CS(=O)(=O)C=C
Mol. weight [g/mol]:	118.15
CAS:	77-77-0

Physical Properties

Property code	Value	Unit	Source
chl	-2826.50 ± 3.50	kJ/mol	NIST Webbook
gf	-310.06	kJ/mol	Joback Method
hf	-156.60 ± 5.00	kJ/mol	NIST Webbook
hf	-151.00 ± 4.00	kJ/mol	NIST Webbook
hfl	-213.00 ± 4.50	kJ/mol	NIST Webbook
hfl	-207.10 ± 3.80	kJ/mol	NIST Webbook
hfus	14.93	kJ/mol	Joback Method
hvap	56.40 ± 0.90	kJ/mol	NIST Webbook
hvap	56.50 ± 0.80	kJ/mol	NIST Webbook
hvap	56.50 ± 0.80	kJ/mol	NIST Webbook
hvap	56.40 ± 0.90	kJ/mol	NIST Webbook
ie	10.56	eV	NIST Webbook
ie	10.62	eV	NIST Webbook
log10ws	-1.03		Crippen Method
logp	0.688		Crippen Method
mcvol	86.710	ml/mol	McGowan Method
pc	5382.80	kPa	Joback Method
tb	332.06	K	Joback Method
tc	501.69	K	Joback Method
tf	169.88	K	Joback Method

vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.93	J/mol×K	332.06	Joback Method
cpg	140.28	J/mol×K	360.33	Joback Method
cpg	147.36	J/mol×K	388.60	Joback Method
cpg	154.18	J/mol×K	416.87	Joback Method
cpg	160.73	J/mol×K	445.15	Joback Method
cpg	167.02	J/mol×K	473.42	Joback Method
cpg	173.06	J/mol×K	501.69	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77770&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

Legend

chl: Standard liquid enthalpy of combustion
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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume