Diethyl sulfone

Other names:	(C2H5)2SO2
	1,1'-Sulphonylbisethane
	Diethyl sulphone
	Ethane, 1,1'-sulfonylbis-
	Ethyl sulfone
Inchi:	InChI=1S/C4H10O2S/c1-3-7(5,6)4-2/h3-4H2,1-2H3
InchiKey:	MBDUIEKYVPVZJH-UHFFFAOYSA-N
Formula:	C4H10O2S
SMILES:	CCS(=O)(=O)CC
Mol. weight [g/mol]:	122.19
CAS:	597-35-3

Physical Properties

Property code	Value	Unit	Source
chs	-3090.00 ± 0.42	kJ/mol	NIST Webbook
gf	-485.74	kJ/mol	Joback Method
hf	-429.30 ± 2.60	kJ/mol	NIST Webbook
hfs	-515.51 ± 0.67	kJ/mol	NIST Webbook
hfus	17.49	kJ/mol	Joback Method
hvap	43.13	kJ/mol	Joback Method
ie	9.96 ± 0.03	eV	NIST Webbook
log10ws	0.04		Aqueous Solubility Prediction Method
logp	0.441		Crippen Method
mcvol	95.310	ml/mol	McGowan Method
pc	4775.98	kPa	Joback Method
tb	338.70	K	Joback Method
tc	501.46	K	Joback Method
tf	345.00 ± 2.00	K	NIST Webbook
tf	345.20 ± 1.00	K	NIST Webbook
tf	346.70 ± 1.50	K	NIST Webbook
tf	347.00 ± 2.00	K	NIST Webbook
tf	345.90	K	Aqueous Solubility Prediction Method
tf	342.20 ± 0.50	K	NIST Webbook
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.13	J/mol×K	338.70	Joback Method
cpg	166.73	J/mol×K	365.83	Joback Method
cpg	175.10	J/mol×K	392.95	Joback Method
cpg	183.24	J/mol×K	420.08	Joback Method
cpg	191.13	J/mol×K	447.21	Joback Method
cpg	198.79	J/mol×K	474.33	Joback Method
cpg	206.20	J/mol×K	501.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50304e+01
Coeff. B	-4.50968e+03
Coeff. C	-8.60300e+01
Temperature range (K), min.	391.92
Temperature range (K), max.	550.04

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C597353&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid 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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume