Sulfuryl fluoride

Other names:	Fluorure de sulfuryle
	SO2F2
	Sulfonyl fluoride
	Sulfur difluoride dioxide
	Sulfur dioxide difluoride
	Sulfur fluoride oxide (SO2F2)
	Sulfuric oxyfluoride
	Sulphuryl fluoride
	UN 2191
	Vikane
	Vikane fumigant
	sulfuryl difluoride
	sulphuryl difluoride
Inchi:	InChI=1S/F2O2S/c1-5(2,3)4
InchiKey:	OBTWBSRJZRCYQV-UHFFFAOYSA-N
Formula:	F2O2S
SMILES:	O=S(=O)(F)F
Mol. weight [g/mol]:	102.06
CAS:	2699-79-8

Physical Properties

Property code	Value	Unit	Source
affp	605.50	kJ/mol	NIST Webbook
basg	580.50	kJ/mol	NIST Webbook
ea	0.77 ± 0.33	eV	NIST Webbook
ea	3.08	eV	NIST Webbook
gf	-909.04	kJ/mol	Joback Method
hf	-888.90	kJ/mol	Joback Method
hfus	13.29	kJ/mol	Joback Method
hvap	32.59	kJ/mol	Joback Method
ie	13.04 ± 0.01	eV	NIST Webbook
ie	13.30 ± 0.10	eV	NIST Webbook
ie	13.04 ± 0.01	eV	NIST Webbook
ie	13.75	eV	NIST Webbook
ie	13.43	eV	NIST Webbook
ie	13.55	eV	NIST Webbook
ie	13.00	eV	NIST Webbook

ie	13.75	eV	NIST Webbook
log10ws	-0.34		Crippen Method
logp	0.170		Crippen Method
mcvol	42.490	ml/mol	McGowan Method
pc	7522.14	kPa	Joback Method
tb	245.72	K	Joback Method
tc	383.59	K	Joback Method
tf	129.50	K	Joback Method
vc	0.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	74.70	J/mol×K	360.61	Joback Method
cpg	65.78	J/mol×K	245.72	Joback Method
cpg	67.56	J/mol×K	268.70	Joback Method
cpg	69.35	J/mol×K	291.68	Joback Method
cpg	71.14	J/mol×K	314.66	Joback Method
cpg	72.92	J/mol×K	337.64	Joback Method
cpg	76.47	J/mol×K	383.59	Joback Method
hvapt	20.00	kJ/mol	196.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38890e+01
Coeff. B	-1.80592e+03
Coeff. C	-2.31500e+01
Temperature range (K), min.	152.00
Temperature range (K), max.	241.00

Sources

Solubilities of sulfuryl fluoride in propylene carbonate, tributyl phosphate and N-methylpyrrolidone:	https://www.doi.org/10.1016/j.jct.2018.05.007
Solubilities of Sulfuryl Fluoride in 2-Butoxyethyl Acetate, 3-Methoxybutyl Acetate, 2-Methoxyethyl Acetate, 1-Methoxy-2-propyl Acetate, and 2-(2-Ethoxyethoxy)ethyl Acetate:	https://www.doi.org/10.1021/acs.jced.8b00224
Solubility and thermodynamic properties of sulfuryl fluoride in water: Crippen Method:	https://www.doi.org/10.1016/j.jct.2015.12.013
	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2699798&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
hvapt:	Enthalpy of vaporization at a given temperature
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