

Thionyl fluoride

Other names:	Fluorure de thionyle OSF2 SOF2 Sulfur difluoride monoxide Sulfur difluoride oxide Sulfurous oxyfluoride Thionyl difluoride
Inchi:	InChI=1S/F2OS/c1-4(2)3
InchiKey:	LSJNBGSOIVSBBR-UHFFFAOYSA-N
Formula:	F2OS
SMILES:	O=S(F)F
Mol. weight [g/mol]:	86.06
CAS:	7783-42-8

Physical Properties

Property code	Value	Unit	Source
gf	-658.21	kJ/mol	Joback Method
hf	-641.29	kJ/mol	Joback Method
hfus	9.67	kJ/mol	Joback Method
hvap	26.69	kJ/mol	Joback Method
ie	12.58	eV	NIST Webbook
ie	12.70	eV	NIST Webbook
ie	12.19	eV	NIST Webbook
ie	12.25 ± 0.05	eV	NIST Webbook
ie	12.60	eV	NIST Webbook
ie	12.25	eV	NIST Webbook
ie	12.58 ± 0.10	eV	NIST Webbook
ie	12.30	eV	NIST Webbook
ie	12.58	eV	NIST Webbook
log10ws	-0.15		Crippen Method
logp	0.504		Crippen Method
mcvol	36.620	ml/mol	McGowan Method
pc	6696.65	kPa	Joback Method
tb	232.50 ± 2.50	K	NIST Webbook
tc	407.76	K	Joback Method
tf	127.42	K	Joback Method
vc	0.162	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	54.21	J/mol×K	256.22	Joback Method
cpg	55.61	J/mol×K	281.48	Joback Method
cpg	57.01	J/mol×K	306.73	Joback Method
cpg	58.41	J/mol×K	331.99	Joback Method
cpg	59.81	J/mol×K	357.25	Joback Method
cpg	61.20	J/mol×K	382.50	Joback Method
cpg	62.59	J/mol×K	407.76	Joback Method
hvapt	23.70	kJ/mol	208.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.24542e+01
Coeff. B	-1.31083e+03
Coeff. C	-6.20600e+01
Temperature range (K), min.	174.42
Temperature range (K), max.	229.35

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7783428&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
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

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