trichlorotrifluoroethane

Other names:	1,1,1-trichloro-2,2,2-trifluoroethane
	1,1,1-trichlorotrifluoroethane
	1,1,1-trifluoro-2,2,2-trichloroethane
	1,1,1-trifluorotrichloroethane
	2,2,2-Trichloro-1,1,1-trifluoro-ethane
	CF3CCl3
	CFC 113a
	F 113a
	FC 113a
	Freon FT
	Freon-FT
	Precision cleaning agent
	R-113a
	T-WD602
	ethane, 1,1,1-trichloro-2,2,2-trifluoro-
	freon 113a
Inchi:	InChI=1S/C2Cl3F3/c3-1(4,5)2(6,7)8
InchiKey:	BOSAWIQFTJIYIS-UHFFFAOYSA-N
Formula:	C2Cl3F3
SMILES:	FC(F)(F)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	187.38
CAS:	26523-64-8

Physical Properties

Property code	Value	Unit	Source
af	0.2351		Cheméo Relay (1.0)
gf	-648.58	kJ/mol	Joback Method
hf	-708.23	kJ/mol	Cheméo Relay (1.0)
hfus	7.94	kJ/mol	Joback Method
hvap	26.58	kJ/mol	Cheméo Relay (1.0)
ie	11.91	eV	Cheméo Relay (1.0)
log10ws	-2.50		Cheméo Relay (1.0)
logp	2.919		Crippen Method
mcvol	81.070	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method

tb	319.15	K	Vapor Liquid Equilibrium for the 1,1,1-Trifluorotrichloroethane + Sulfuryl Chloride System at 101.3 kPa
tc	480.52	K	Cheméo Relay (1.0)
tf	288.38	K	Cheméo Relay (1.0)
vc	0.304	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.81	J/mol×K	348.80	Joback Method
cpg	132.62	J/mol×K	379.64	Joback Method
cpg	137.83	J/mol×K	410.49	Joback Method
cpg	142.49	J/mol×K	441.33	Joback Method
cpg	146.63	J/mol×K	472.18	Joback Method
cpg	150.28	J/mol×K	503.02	Joback Method
cpg	153.48	J/mol×K	533.87	Joback Method
hvapt	30.50	kJ/mol	300.00	NIST Webbook
pvap	101.30	kPa	319.15	Vapor Liquid Equilibrium for the 1,1,1-Trifluorotrichloroethane + Sulfuryl Chloride System at 101.3 kPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48158e+01
Coeff. B	-3.05174e+03
Coeff. C	-1.95350e+01
Temperature range (K), min.	229.59
Temperature range (K), max.	341.35

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor Liquid Equilibrium for the 1,1,1-Trifluorotrichloroethane + Sulfuryl Chloride System at 101.3 kPa:	https://www.doi.org/10.1021/je400544h
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility Differences of Halocarbon Isomers in Ionic Liquid [emim][Tf2N]:	https://www.doi.org/10.1021/je700295e
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26523648&Units=SI

Legend

af:	Acentric Factor
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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