

Methanethiol, trifluoro-

Other names:	Perfluoromethanethiol Trifluoromethanethiol Trifluoromethylmercaptan
Inchi:	InChI=1S/CHF3S/c2-1(3,4)5/h5H
InchiKey:	MFLLMKMFWIUACU-UHFFFAOYSA-N
Formula:	CHF3S
SMILES:	FC(F)(F)S
Mol. weight [g/mol]:	102.08
CAS:	1493-15-8

Physical Properties

Property code	Value	Unit	Source
gf	-594.66	kJ/mol	Joback Method
hf	-622.57	kJ/mol	Joback Method
hfus	4.21	kJ/mol	Joback Method
hvap	20.81	kJ/mol	Joback Method
ie	11.40 ± 0.10	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.436		Crippen Method
mcvol	46.610	ml/mol	McGowan Method
pc	5359.18	kPa	Joback Method
sl	204.60	J/mol×K	NIST Webbook
tb	279.72	K	Joback Method
tc	448.46	K	Joback Method
tf	141.68	K	Joback Method
vc	0.189	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	71.67	J/mol×K	279.72	Joback Method
cpg	90.08	J/mol×K	420.34	Joback Method
cpg	86.93	J/mol×K	392.21	Joback Method
cpg	83.54	J/mol×K	364.09	Joback Method

cpg	79.87	J/mol×K	335.97	Joback Method
cpg	75.92	J/mol×K	307.84	Joback Method
cpg	92.98	J/mol×K	448.46	Joback Method
cpl	113.09	J/mol×K	235.00	NIST Webbook
hfust	4.93	kJ/mol	116.00	NIST Webbook
hfust	4.93	kJ/mol	116.00	NIST Webbook
hfust	4.92	kJ/mol	116.04	NIST Webbook
hvapt	21.00	kJ/mol	201.50	NIST Webbook
hvapt	21.80	kJ/mol	201.50	NIST Webbook
sfust	42.43	J/mol×K	116.04	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44027e+01
Coeff. B	-2.11988e+03
Coeff. C	-1.85100e+01
Temperature range (K), min.	168.00
Temperature range (K), max.	251.69

Sources

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=C1493158&Units=SI
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/ci990307I

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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