Acetonitrile, trifluoro-

Other names:	CF3CN
	CYANOTRIFLUOROMETHANE
	TRIFLUOROACETONITRILE
Inchi:	InChI=1S/C2F3N/c3-2(4,5)1-6
InchiKey:	SFFUEHODRAXXIA-UHFFFAOYSA-N
Formula:	C2F3N
SMILES:	N#CC(F)(F)F
Mol. weight [g/mol]:	95.02
CAS:	353-85-5

Physical Properties

Property code	Value	Unit	Source
af	0.2670		KDB
affp	688.40	kJ/mol	NIST Webbook
basg	657.70	kJ/mol	NIST Webbook
gf	-462.20	kJ/mol	KDB
hf	-496.60 ± 0.63	kJ/mol	NIST Webbook
hf	-460.00 ± 30.00	kJ/mol	NIST Webbook
hf	-495.70	kJ/mol	KDB
hfus	4.27	kJ/mol	Joback Method
hvap	26.78	kJ/mol	Joback Method
ie	13.93 ± 0.07	eV	NIST Webbook
ie	13.86	eV	NIST Webbook
ie	14.30	eV	NIST Webbook
ie	14.00	eV	NIST Webbook
log10ws	-1.19		Crippen Method
logp	1.072		Crippen Method
mcvol	45.730	ml/mol	McGowan Method
pc	3618.00	kPa	KDB
pc	3618.00 ± 3.44	kPa	NIST Webbook
rhoc	470.37 ± 4.69	kg/m3	NIST Webbook
rinpol	246.00		NIST Webbook
rinpol	246.00		NIST Webbook
sl	184.43	J/mol×K	NIST Webbook
tb	209.00	K	NIST Webbook
tb	204.33	K	KDB
tb	209.00	K	NIST Webbook

tc	311.11	K	KDB
tc	311.11 ± 0.20	K	NIST Webbook
tf	181.48	K	Joback Method
tt	128.73 ± 0.02	K	NIST Webbook
vc	0.202	m3/kmol	KDB
zc	0.2825330		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	96.03	J/mol×K	457.94	Joback Method
cpg	98.75	J/mol×K	486.97	Joback Method
cpg	82.59	J/mol×K	341.82	Joback Method
cpg	86.37	J/mol×K	370.85	Joback Method
cpg	89.86	J/mol×K	399.88	Joback Method
cpg	93.07	J/mol×K	428.91	Joback Method
cpg	101.24	J/mol×K	516.00	Joback Method
cpl	118.11	J/mol×K	205.00	NIST Webbook
hfust	4.97	kJ/mol	128.70	NIST Webbook
hfust	4.97	kJ/mol	128.73	NIST Webbook
hfust	4.97	kJ/mol	128.70	NIST Webbook
hvapt	17.83	kJ/mol	205.47	NIST Webbook
hvapt	19.20	kJ/mol	174.00	NIST Webbook
hvapt	19.30	kJ/mol	178.50	NIST Webbook
hvapt	19.20	kJ/mol	172.00	NIST Webbook
hvapt	18.50	kJ/mol	219.00	NIST Webbook
hvapt	17.40	kJ/mol	309.00	NIST Webbook
hvapt	17.40	kJ/mol	291.50	NIST Webbook
sfust	38.62	J/mol×K	128.73	NIST Webbook
svapt	86.79	J/mol×K	205.47	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56198e+01
Coeff. B	-2.13202e+03

Coeff. C	-1.05560e+01
Temperature range (K), min.	147.05
Temperature range (K), max.	217.38

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C353855&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1770
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
rhoc:	Critical density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
svapt:	Entropy of vaporization at a given temperature

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility