

Nitrogen trifluoride

Other names:	NF3 Nitrogen fluoride Nitrogen fluoride (NF3) PERFLUOROAMMONIA TRIFLUOROAMINE TRIFLUOROAMMONIA UN 2451
Inchi:	InChI=1S/F3N/c1-4(2)3
InchiKey:	GVGCUCJTUSOZKP-UHFFFAOYSA-N
Formula:	F3N
SMILES:	FN(F)F
Mol. weight [g/mol]:	71.00
CAS:	7783-54-2

Physical Properties

Property code	Value	Unit	Source
af	0.1350		KDB
affp	568.40	kJ/mol	NIST Webbook
basg	554.00	kJ/mol	NIST Webbook
basg	538.60	kJ/mol	NIST Webbook
dm	0.20	debye	KDB
gf	-90.10	kJ/mol	KDB
hf	-131.60	kJ/mol	KDB
hfus	8.02	kJ/mol	Joback Method
hvap	15.19	kJ/mol	Joback Method
ie	12.94 ± 0.01	eV	NIST Webbook
ie	13.83	eV	NIST Webbook
ie	13.60 ± 0.20	eV	NIST Webbook
ie	13.75	eV	NIST Webbook
ie	13.00 ± 0.02	eV	NIST Webbook
ie	13.20 ± 0.10	eV	NIST Webbook
ie	12.97 ± 0.04	eV	NIST Webbook
ie	13.10 ± 0.06	eV	NIST Webbook
ie	13.73	eV	NIST Webbook
ie	13.00	eV	NIST Webbook
ie	12.94 ± 0.01	eV	NIST Webbook
ie	13.50 ± 0.20	eV	NIST Webbook

ie	13.73 ± 0.03	eV	NIST Webbook
log10ws	-0.92		Crippen Method
logp	0.942		Crippen Method
mcvol	26.150	ml/mol	McGowan Method
pc	4460.00	kPa	KDB
tb	144.40	K	KDB
tb	144.00 ± 1.50	K	NIST Webbook
tb	144.20 ± 0.40	K	NIST Webbook
tc	234.00	K	KDB
tf	66.36	K	KDB
tf	64.70 ± 0.50	K	NIST Webbook
vc	0.126	m3/kmol	KDB
zc	0.2888370		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	38.99	J/mol×K	209.65	Joback Method
cpg	41.22	J/mol×K	230.18	Joback Method
cpg	43.36	J/mol×K	250.71	Joback Method
cpg	45.41	J/mol×K	271.23	Joback Method
cpg	47.38	J/mol×K	291.76	Joback Method
cpg	49.26	J/mol×K	312.29	Joback Method
cpg	51.05	J/mol×K	332.82	Joback Method
rhoI	1540.00	kg/m3	144.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41411e+01
Coeff. B	-1.28834e+03
Coeff. C	-8.80000e+00
Temperature range (K), min.	66.36
Temperature range (K), max.	233.85

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1903.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7783542&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

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
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
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
rho:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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