2,2,2-Trifluoroethylamine

Other names:	CF3CH2NH2
	Ethanamine, 2,2,2-trifluoro-
	Ethylamine, 2,2,2-trifluoro-
	Trifluoroethylamine
	«beta»,«beta»,«beta»-Trifluoroethylamine
	Â«betaÂ»,Â«betaÂ»,Â«betaÂ»-Trifluoroethylamine
Inchi:	InChI=1S/C2H4F3N/c3-2(4,5)1-6/h1,6H2
InchiKey:	KIPSRYDSZQRPEA-UHFFFAOYSA-N
Formula:	C2H4F3N
SMILES:	NCC(F)(F)F
Mol. weight [g/mol]:	99.06
CAS:	753-90-2

Physical Properties

Property code	Value	Unit	Source
affp	846.80	kJ/mol	NIST Webbook
basg	812.90	kJ/mol	NIST Webbook
gf	-549.18	kJ/mol	Joback Method
hf	-647.90	kJ/mol	Joback Method
hfus	7.96	kJ/mol	Joback Method
hvap	26.94	kJ/mol	Joback Method
ie	9.70	eV	NIST Webbook
ie	9.97	eV	NIST Webbook
log10ws	-0.76		Crippen Method
logp	0.507		Crippen Method
mcvol	54.330	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
tb	309.00	K	NIST Webbook
tb	309.20	K	NIST Webbook
tb	310.70	K	NIST Webbook
tc	475.03	K	Joback Method
tf	199.75	K	Joback Method
vc	0.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.90	J/mol×K	312.27	Joback Method
cpg	107.00	J/mol×K	339.40	Joback Method
cpg	112.76	J/mol×K	366.52	Joback Method
cpg	118.18	J/mol×K	393.65	Joback Method
cpg	123.29	J/mol×K	420.78	Joback Method
cpg	128.09	J/mol×K	447.91	Joback Method
cpg	132.60	J/mol×K	475.03	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol1770.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C753902&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity
basg: Gas basicity
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume