Methane, trifluoronitro-

Other names: Trifluoronitromethane
Inchi: InChI=1S/CF3NO2/c2-1(3,4)5(6)7
InchiKey: GEGIENATMYITAP-UHFFFAOYSA-N
Formula: CF3NO2
SMILES: O=[N+]([O-])C(F)(F)F
Mol. weight [g/mol]: 115.01
CAS: 335-02-4

Physical Properties

Property code	Value	Unit	Source
gf	-588.50	kJ/mol	Joback Method
hf	-671.81	kJ/mol	Joback Method
hfus	11.53	kJ/mol	Joback Method
hvap	30.66	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	0.783		Crippen Method
mcvol	47.680	ml/mol	McGowan Method
pc	4973.33	kPa	Joback Method
rinpol	318.00		NIST Webbook
tb	368.70	K	Joback Method
tc	560.53	K	Joback Method
tf	248.83	K	Joback Method
vc	0.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.14	J/mol×K	528.56	Joback Method
cpg	94.38	J/mol×K	368.70	Joback Method
cpg	99.30	J/mol×K	400.67	Joback Method
cpg	103.82	J/mol×K	432.64	Joback Method
cpg	107.95	J/mol×K	464.62	Joback Method
cpg	111.72	J/mol×K	496.59	Joback Method
cpg	118.25	J/mol×K	560.53	Joback Method

hvapt	21.60	kJ/mol	240.50	NIST Webbook

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=C335024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume