2-Propenenitrile, 2,3,3-trifluoro-

Other names: Acrylonitrile, trifluoro-
Perfluoroacrylonitrile
CF2=CFCN
Inchi: InChI=1S/C3F3N/c4-2(1-7)3(5)6
InchiKey: KDUAIKFAYXQCMF-UHFFFAOYSA-N
Formula: C3F3N
SMILES: N#CC(F)=C(F)F
Mol. weight [g/mol]: 107.03
CAS: 433-43-2

Physical Properties

Property code	Value	Unit	Source
gf	-413.75	kJ/mol	Joback Method
hf	-431.06	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	30.42	kJ/mol	Joback Method
ie	10.60 ± 0.10	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	1.588		Crippen Method
mcvol	55.520	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
tb	371.85	K	Joback Method
tc	550.66	K	Joback Method
tf	157.33	K	Joback Method
vc	0.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	95.95	J/mol×K	371.85	Joback Method
cpg	99.74	J/mol×K	401.65	Joback Method
cpg	103.27	J/mol×K	431.45	Joback Method
cpg	106.57	J/mol×K	461.26	Joback Method
cpg	109.64	J/mol×K	491.06	Joback Method

cpg	112.50	J/mol×K	520.86	Joback Method
cpg	115.16	J/mol×K	550.66	Joback Method

Sources

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=C433432&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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