1-Fluoropropenenitrile

Inchi: InChI=1S/C3H2FN/c4-2-1-3-5/h1-2H/b2-1+
InchiKey: DOERUWDOBMTXGO-OWOJBTEDSA-N
Formula: C3H2FN
SMILES: N#CC=CF
Mol. weight [g/mol]: 71.05
CAS: 430-49-9

Physical Properties

Property code	Value	Unit	Source
gf	-7.03	kJ/mol	Joback Method
hf	-19.26	kJ/mol	Joback Method
hfus	8.31	kJ/mol	Joback Method
hvap	31.89	kJ/mol	Joback Method
ie	10.70 ± 0.10	eV	NIST Webbook
log10ws	-1.15		Crippen Method
logp	0.993		Crippen Method
mcvol	51.980	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
tb	373.55	K	Joback Method
tc	565.99	K	Joback Method
tf	184.07	K	Joback Method
vc	0.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	79.08	J/mol×K	373.55	Joback Method
cpg	83.10	J/mol×K	405.62	Joback Method
cpg	86.86	J/mol×K	437.70	Joback Method
cpg	90.40	J/mol×K	469.77	Joback Method
cpg	93.70	J/mol×K	501.85	Joback Method
cpg	96.80	J/mol×K	533.92	Joback Method
cpg	99.71	J/mol×K	565.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C430499&Units=SI
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

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