

2-Propynenitrile, 3-fluoro-

Other names:	CF«equiv»CCN
Inchi:	InChI=1S/C3FN/c4-2-1-3-5
InchiKey:	RBVSYFWRRIFVAC-UHFFFAOYSA-N
Formula:	C3FN
SMILES:	N#CC#CF
Mol. weight [g/mol]:	69.04
CAS:	32038-83-8

Physical Properties

Property code	Value	Unit	Source
gf	115.55	kJ/mol	Joback Method
hf	135.82	kJ/mol	Joback Method
hfus	11.23	kJ/mol	Joback Method
hvap	34.09	kJ/mol	Joback Method
ie	11.51 ± 0.02	eV	NIST Webbook
log10ws	-1.09		Crippen Method
logp	0.440		Crippen Method
mcvol	47.680	ml/mol	McGowan Method
pc	4987.39	kPa	Joback Method
tb	378.39	K	Joback Method
tc	589.16	K	Joback Method
tf	295.25	K	Joback Method
vc	0.209	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	68.67	J/mol×K	378.39	Joback Method
cpg	70.82	J/mol×K	413.52	Joback Method
cpg	72.89	J/mol×K	448.65	Joback Method
cpg	74.89	J/mol×K	483.78	Joback Method
cpg	76.82	J/mol×K	518.91	Joback Method
cpg	78.68	J/mol×K	554.03	Joback Method
cpg	80.47	J/mol×K	589.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32038838&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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