

Difluorocyanamide

Inchi:	InChI=1S/CF2N2/c2-5(3)1-4
InchiKey:	HFFQLQRGCQEGJG-UHFFFAOYSA-N
Formula:	CF2N2
SMILES:	N#CN(F)F
Mol. weight [g/mol]:	78.02
CAS:	7127-18-6

Physical Properties

Property code	Value	Unit	Source
gf	-188.12	kJ/mol	Joback Method
hf	-223.78	kJ/mol	Joback Method
hfus	9.03	kJ/mol	Joback Method
hvap	28.71	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.538		Crippen Method
mcvol	39.850	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	335.34	K	Joback Method
tc	506.76	K	Joback Method
tf	199.67	K	Joback Method
vc	0.172	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	66.52	J/mol×K	335.34	Joback Method
cpg	69.24	J/mol×K	363.91	Joback Method
cpg	71.81	J/mol×K	392.48	Joback Method
cpg	74.23	J/mol×K	421.05	Joback Method
cpg	76.49	J/mol×K	449.62	Joback Method
cpg	78.62	J/mol×K	478.19	Joback Method
cpg	80.60	J/mol×K	506.76	Joback Method
hvapt	20.60	kJ/mol	188.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63368e+01
Coeff. B	-2.47528e+03
Temperature range (K), min.	154.23
Temperature range (K), max.	224.51

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7127186&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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