2,2=Difluoropropenenitrile

Inchi: InChI=1S/C3HF2N/c4-3(5)1-2-6/h1H
InchiKey: PSUCPEMMGCPVFE-UHFFFAOYSA-N
Formula: C3HF2N
SMILES: N#CC=C(F)F
Mol. weight [g/mol]: 89.04
CAS: 461-51-8

Physical Properties

Property code	Value	Unit	Source
gf	-210.39	kJ/mol	Joback Method
hf	-225.16	kJ/mol	Joback Method
hfus	10.08	kJ/mol	Joback Method
hvap	31.15	kJ/mol	Joback Method
ie	10.60 ± 0.10	eV	NIST Webbook
log10ws	-1.50		Crippen Method
logp	1.290		Crippen Method
mcvol	53.750	ml/mol	McGowan Method
pc	4088.15	kPa	Joback Method
tb	372.70	K	Joback Method
tc	558.16	K	Joback Method
tf	170.70	K	Joback Method
vc	0.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	87.51	J/mol×K	372.70	Joback Method
cpg	91.41	J/mol×K	403.61	Joback Method
cpg	95.06	J/mol×K	434.52	Joback Method
cpg	98.47	J/mol×K	465.43	Joback Method
cpg	101.66	J/mol×K	496.34	Joback Method
cpg	104.63	J/mol×K	527.25	Joback Method
cpg	107.41	J/mol×K	558.16	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C461518&Units=SI

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