2-Butynenitrile, 4,4,4-trifluoro-

Inchi: InChI=1S/C4F3N/c5-4(6,7)2-1-3-8
InchiKey: YZNFAKUUGQFZOK-UHFFFAOYSA-N
Formula: C4F3N
SMILES: N#CC#CC(F)(F)F
Mol. weight [g/mol]: 119.04
CAS: 66051-48-7

Physical Properties

Property code	Value	Unit	Source
gf	-262.81	kJ/mol	Joback Method
hf	-285.79	kJ/mol	Joback Method
hfus	12.57	kJ/mol	Joback Method
hvap	33.38	kJ/mol	Joback Method
ie	12.00	eV	NIST Webbook
ie	12.00 ± 0.02	eV	NIST Webbook
ie	12.26	eV	NIST Webbook
log10ws	-1.82		Crippen Method
logp	1.076		Crippen Method
mcvol	65.310	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	396.58	K	Joback Method
tc	595.86	K	Joback Method
tf	310.12	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.71	J/mol×K	396.58	Joback Method
cpg	123.33	J/mol×K	429.79	Joback Method
cpg	127.58	J/mol×K	463.01	Joback Method
cpg	131.49	J/mol×K	496.22	Joback Method
cpg	135.08	J/mol×K	529.43	Joback Method
cpg	138.37	J/mol×K	562.64	Joback Method

cpg	141.38	J/mol×K	595.86	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=C66051487&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