Tetrafluorophthalonitrile

Other names:	1,2-Benzenedicarbonitrile, 3,4,5,6-tetrafluoro- 3,4,5,6-tetrafluorobenzene-1,2-dicarbonitrile
Inchi:	InChI=1S/C8F4N2/c9-5-3(1-13)4(2-14)6(10)8(12)7(5)11
InchiKey:	OFLRJMBSWDXSPG-UHFFFAOYSA-N
Formula:	C8F4N2
SMILES:	N#Cc1c(F)c(F)c(F)c(F)c1C#N
Mol. weight [g/mol]:	200.09
CAS:	1835-65-0

Physical Properties

Property code	Value	Unit	Source
gf	-432.14	kJ/mol	Joback Method
hf	-483.95	kJ/mol	Joback Method
hfus	23.90	kJ/mol	Joback Method
hvap	56.68	kJ/mol	Joback Method
ie	10.60	eV	NIST Webbook
log10ws	-3.50		Crippen Method
logp	1.986		Crippen Method
mcvol	109.660	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
tb	635.26	K	Joback Method
tc	843.92	K	Joback Method
tf	401.28	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.69	J/mol×K	635.26	Joback Method
cpg	244.00	J/mol×K	670.04	Joback Method
cpg	249.01	J/mol×K	704.81	Joback Method
cpg	253.73	J/mol×K	739.59	Joback Method
cpg	258.16	J/mol×K	774.37	Joback Method
cpg	262.28	J/mol×K	809.15	Joback Method

cpg	266.11	J/mol×K	843.92	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=C1835650&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