Benzonitrile, pentafluoro-

Other names:	Pentafluorobenzonitrile
	Perfluorobenzonitrile
	2,3,4,5,6-Pentafluorobenzonitrile
	Pentafluorocyanobenzene
	Cyanopentafluorobenzene
Inchi:	InChI=1S/C7F5N/c8-3-2(1-13)4(9)6(11)7(12)5(3)10
InchiKey:	YXWJGZQOGXGSSC-UHFFFAOYSA-N
Formula:	C7F5N
SMILES:	N#Cc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	193.07
CAS:	773-82-0

Physical Properties

Property code	Value	Unit	Source
ea	1.08 ± 0.11	eV	NIST Webbook
gf	-768.55	kJ/mol	Joback Method
hf	-824.30	kJ/mol	Joback Method
hfus	22.89	kJ/mol	Joback Method
hvap	43.16	kJ/mol	Joback Method
ie	10.10	eV	NIST Webbook
ie	10.45	eV	NIST Webbook
log10ws	-3.48		Crippen Method
logp	2.254		Crippen Method
mcvol	95.960	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	435.20	K	NIST Webbook
tb	435.00	K	NIST Webbook
tc	696.35	K	Joback Method
tf	325.61	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	199.72	J/mol×K	509.57	Joback Method
cpg	205.09	J/mol×K	540.70	Joback Method
cpg	210.25	J/mol×K	571.83	Joback Method
cpg	215.19	J/mol×K	602.96	Joback Method
cpg	219.91	J/mol×K	634.09	Joback Method
cpg	224.40	J/mol×K	665.22	Joback Method
cpg	228.68	J/mol×K	696.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C773820&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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

Latest version available from:
https://www.chemeo.com/cid/28-125-2/Benzonitrile-pentafluoro.pdf
Generated by Cheméo on 2024-10-12 04:40:42.727737144 +0000 UTC m=+3288905.364706394.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.