Benzonitrile, 4-(trifluoromethyl)-

Other names:	p-Cyanobenzotrifluoride
	p-Tolunitrile, «alpha»,«alpha»,«alpha»-trifluoro-
	p-(Trifluoromethyl)benzonitrile
	4-Trifluoromethylbenzonitrile
	«alpha»,«alpha»,«alpha»-Trifluoro-p-toluonitrile
	Benzonitrile, p-(trifluoromethyl)-
	p-Tolunitrile, alpha,alpha,alpha-trifluoro-
	4-Trifluoromethylbenzoic acid nitrile
	«alpha»,«alpha»,«alpha»-trifluoro-4-toluonitrile
Inchi:	InChI=1S/C8H4F3N/c9-8(10,11)7-3-1-6(5-12)2-4-7/h1-4H
InchiKey:	DRNJIKRLQJRKMM-UHFFFAOYSA-N
Formula:	C8H4F3N
SMILES:	N#Cc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	171.12
CAS:	455-18-5

Physical Properties

Property code	Value	Unit	Source
affp	787.20	kJ/mol	NIST Webbook
basg	758.30	kJ/mol	NIST Webbook
ea	0.76 ± 0.09	eV	NIST Webbook
gf	-329.15	kJ/mol	Joback Method
hf	-415.59	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	43.07	kJ/mol	Joback Method
ie	10.61 ± 0.05	eV	NIST Webbook
log10ws	-2.93		Crippen Method
logp	2.577		Crippen Method
mcvol	106.510	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
tb	510.76	K	Joback Method
tc	722.52	K	Joback Method
tf	288.04	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.98	J/mol×K	510.76	Joback Method
cpg	239.29	J/mol×K	546.05	Joback Method
cpg	247.87	J/mol×K	581.35	Joback Method
cpg	255.76	J/mol×K	616.64	Joback Method
cpg	263.01	J/mol×K	651.93	Joback Method
cpg	269.67	J/mol×K	687.23	Joback Method
cpg	275.78	J/mol×K	722.52	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.70	K	2.70	NIST Webbook
tbrp	353.50 ± 0.50	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C455185&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

affp: Proton affinity
basg: Gas basicity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume