5-Amino-2-cyanobenzotrifluoride

Other names:	5-Aminno-2-cyanobenzotrifluoride
	Benzonitrile, 4-amino-2-(trifluoromethyl)-
	4-ciano-3-trifluormetil-anilin
Inchi:	InChI=1S/C8H5F3N2/c9-8(10,11)7-3-6(13)2-1-5(7)4-12/h1-3H,13H2
InchiKey:	PMDYLCUKSLBUHO-UHFFFAOYSA-N
Formula:	C8H5F3N2
SMILES:	N#Cc1ccc(N)cc1C(F)(F)F
Mol. weight [g/mol]:	186.13
CAS:	654-70-6

Physical Properties

Property code	Value	Unit	Source
gf	-272.33	kJ/mol	Joback Method
hf	-393.27	kJ/mol	Joback Method
hfus	18.27	kJ/mol	Joback Method
hvap	54.37	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.159		Crippen Method
mcvol	116.490	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	588.27	K	Joback Method
tc	810.13	K	Joback Method
tf	383.82	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.02	J/mol×K	588.27	Joback Method
cpg	285.72	J/mol×K	625.25	Joback Method
cpg	293.73	J/mol×K	662.22	Joback Method
cpg	301.08	J/mol×K	699.20	Joback Method
cpg	307.83	J/mol×K	736.17	Joback Method
cpg	314.02	J/mol×K	773.15	Joback Method

cpg	319.71	J/mol×K	810.13	Joback Method

Sources

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=C654706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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