Benzonitrile, 3,5-bis(trifluoromethyl)-

Other names:	3,5-di(Trifluoromethyl)benzonitrile
	Bis(3,5-trifluoromethyl)benzonitrile
	Benzonitrile, 3,5-bis(trifluoromethyl)-
	3,5-Bis(trifluoromethyl)-1-cyanobenzene
Inchi:	InChI=1S/C9H3F6N/c10-8(11,12)6-1-5(4-16)2-7(3-6)9(13,14)15/h1-3H
InchiKey:	CZKHHAOIHXHOSR-UHFFFAOYSA-N
Formula:	C9H3F6N
SMILES:	N#Cc1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	239.12

Physical Properties

Property code	Value	Unit	Source
ea	1.14 ± 0.09	eV	NIST Webbook
hfus	17.49	kJ/mol	Joback Method
ie	10.29	eV	Cheméo Relay (1.0)
logp	3.596		Crippen Method
mcvol	125.910	ml/mol	McGowan Method
tb	460.58	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.29	J/mol×K	533.20	Joback Method
cpg	309.50	J/mol×K	565.18	Joback Method
cpg	317.96	J/mol×K	597.16	Joback Method
cpg	325.72	J/mol×K	629.15	Joback Method
cpg	332.84	J/mol×K	661.13	Joback Method
cpg	339.36	J/mol×K	693.11	Joback Method
cpg	345.34	J/mol×K	725.09	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27126938&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature