Benzenamine, 3,5-bis(trifluoromethyl)-

Other names:	3,5-Bis(trifluoromethyl)aniline 3,5-Bis(trifluoromethyl)benzenamine «alpha»,«alpha»,«alpha»,«alpha»',«alpha»',«alpha»'-Hexafluoro-3,5-xylidine 3,5-Xylidine, «alpha»,«alpha»,«alpha»,«alpha»',«alpha»',«alpha»'-hexafluoro- 3,5-di(Trifluoromethyl)aniline Aniline, 3,5-bis(trifluoromethyl)- 3,5-Xylidine, alpha,alpha,alpha,alpha',alpha',alpha'-hexafluoro- alpha,alpha,alpha,alpha',alpha',alpha'-Hexafluoro-3,5-xylidine 3,5-Bis-trifluoromethyl-phenylamine NSC 3411
Inchi:	InChI=1S/C8H5F6N/c9-7(10,11)4-1-5(8(12,13)14)3-6(15)2-4/h1-3H,15H2
InchiKey:	CDIDGWDGQGVCIB-UHFFFAOYSA-N
Formula:	C8H5F6N
SMILES:	Nc1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	229.12
CAS:	328-74-5

Physical Properties

Property code	Value	Unit	Source
gf	-987.10	kJ/mol	Joback Method
hf	-1155.23	kJ/mol	Joback Method
hfus	18.59	kJ/mol	Joback Method
hvap	40.15	kJ/mol	Joback Method
ie	8.59	eV	NIST Webbook
log10ws	-3.31		Crippen Method
logp	3.306		Crippen Method
mcvol	120.420	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1057.80		NIST Webbook
tb	480.77	K	Joback Method
tc	667.48	K	Joback Method
tf	323.02	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.29	J/mol×K	480.77	Joback Method
cpg	296.04	J/mol×K	511.89	Joback Method
cpg	306.00	J/mol×K	543.01	Joback Method
cpg	315.19	J/mol×K	574.13	Joback Method
cpg	323.68	J/mol×K	605.25	Joback Method
cpg	331.50	J/mol×K	636.37	Joback Method
cpg	338.71	J/mol×K	667.48	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.00	K	2.00	NIST Webbook
tbrp	358.20	K	2.00	NIST Webbook
tbrp	358.00	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C328745&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume