Benzenamine, 3-(trifluoromethyl)-

Other names: 1-Amino-3-(trifluoromethyl)benzene
3-(Trifluoromethyl)aniline
3-(Trifluoromethyl)benzenamine
3-Aminobenzotrifluoride
3-Trifluromethylaniline
NSC 4540
Toluene, 3-amino-«alpha»,«alpha»,«alpha»-trifluoro-,
Toluene, 3-amino-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-,
UN 2948
USAF ma-4
m-(Trifluoromethyl)aniline
m-Abtf
m-Amino-«alpha»,«alpha»,«alpha»-trifluorotoluene
m-Amino-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluorotoluene
m-Aminobenzal fluoride
m-Aminobenzotrifluoride
m-Toluidine, «alpha»,«alpha»,«alpha»-trifluoro-
m-Toluidine, Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-
«alpha»,«alpha»,«alpha»-Trifluoro-m-toluidine
Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Trifluoro-m-toluidine

Inchi: InChI=1S/C7H6F3N/c8-7(9,10)5-2-1-3-6(11)4-5/h1-4H,11H2

InchiKey: VIUDTWATMPPKEL-UHFFFAOYSA-N

Formula: C7H6F3N

SMILES: Nc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 161.12

CAS: 98-16-8

Physical Properties

Property code	Value	Unit	Source
affp	856.90	kJ/mol	NIST Webbook
basg	825.10	kJ/mol	NIST Webbook
chl	-3455.00	kJ/mol	NIST Webbook
chl	-3476.70	kJ/mol	NIST Webbook
gf	-404.30	kJ/mol	Joback Method
hf	-526.04	kJ/mol	Joback Method
hfl	-686.01	kJ/mol	NIST Webbook
hfus	14.56	kJ/mol	Joback Method

hvap	41.01	kJ/mol	Joback Method
log10ws	-1.47		Aqueous Solubility Prediction Method
logp	2.288		Crippen Method
mcvol	101.020	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	1017.60		NIST Webbook
rinpol	1017.60		NIST Webbook
tb	460.20	K	NIST Webbook
tb	459.50 ± 0.50	K	NIST Webbook
tc	664.73	K	Joback Method
tf	278.90	K	Aqueous Solubility Prediction Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.15	J/mol×K	458.33	Joback Method
cpg	226.94	J/mol×K	492.73	Joback Method
cpg	236.95	J/mol×K	527.13	Joback Method
cpg	246.21	J/mol×K	561.53	Joback Method
cpg	254.78	J/mol×K	595.93	Joback Method
cpg	262.69	J/mol×K	630.33	Joback Method
cpg	269.98	J/mol×K	664.73	Joback Method
hvapt	53.10	kJ/mol	399.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.80	K	2.70	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46024e+01
Coeff. B	-3.79975e+03
Coeff. C	-7.95700e+01
Temperature range (K), min.	334.00
Temperature range (K), max.	488.54

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98168&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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