Benzenamine, 2-(trifluoromethyl)-

Other names:	o-Toluidine, «alpha»,«alpha»,«alpha»-trifluoro- «alpha»,«alpha»,«alpha»-Trifluoro-o-toluidine o-(Trifluoromethyl)aniline o-Aminobenzotrifluoride 2-(Trifluoromethyl)aniline 2-(Trifluoromethyl)benzenamine 2-Aminobenzotrifluoride 2-Trifluromethylaniline UN 2942 2-Trifluoromethyl-phenylamine NSC 10336 o-(Trifluoromethyl)phenylamine
Inchi:	InChI=1S/C7H6F3N/c8-7(9,10)5-3-1-2-4-6(5)11/h1-4H,11H2
InchiKey:	VBLXCTYLWZJBKA-UHFFFAOYSA-N
Formula:	C7H6F3N
SMILES:	Nc1ccccc1C(F)(F)F
Mol. weight [g/mol]:	161.12
CAS:	88-17-5

Physical Properties

Property code	Value	Unit	Source
gf	-404.30	kJ/mol	Joback Method
hf	-526.04	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	41.01	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.288		Crippen Method
mcvol	101.020	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	955.50		NIST Webbook
tb	458.33	K	Joback Method
tc	664.73	K	Joback Method
tf	295.04	K	Joback 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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	339.00 ± 1.00	K	2.00	NIST Webbook
tbrp	341.20	K	2.00	NIST Webbook
tbrp	340.50 ± 0.50	K	2.00	NIST Webbook

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=C88175&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
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