Benzene, 1-isocyanato-3-(trifluoromethyl)-

Other names:	Isocyanic acid, «alpha»,«alpha»,«alpha»-trifluoro-m-tolyl ester
	m-(Trifluoromethyl)phenyl isocyanate
	3-(Trifluoromethyl)phenyl isocyanate
	«alpha»,«alpha»,«alpha»-Trifluoro-m-tolyl isocyanate
	«alpha»,«alpha»,«alpha»-Trifluoro-3-tolyl isocyanate
	«alpha»,«alpha»,«alpha»-Trifluoro-meta-tolylisocyanate
	Isocyanic acid m-trifluoromethylphenyl ester
Inchi:	InChI=1S/C8H4F3NO/c9-8(10,11)6-2-1-3-7(4-6)12-5-13/h1-4H
InchiKey:	SXJYSIBLFGQAND-UHFFFAOYSA-N
Formula:	C8H4F3NO
SMILES:	O=C=Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	187.12
CAS:	329-01-1

Physical Properties

Property code	Value	Unit	Source
hf	-585.88	kJ/mol	Joback Method
hvap	42.12	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	2.673		Crippen Method
mcvol	112.380	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	475.35	K	Joback Method
tc	677.05	K	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	327.00	K	1.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C329011&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

hf:	Enthalpy of formation 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature