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

Other names:	Isothiocyanic acid, «alpha»,«alpha»,«alpha»-trifluoro-m-tolyl ester
	m-Trifluoromethylphenol isothiocyanate
	m-(Trifluoromethyl)phenyl isothiocyanate
	3-(Trifluoromethyl)phenyl isothiocyanate
	«alpha»,«alpha»,«alpha»-Trifluoro-m-tolyl isothiocyanate
Inchi:	InChI=1S/C8H4F3NS/c9-8(10,11)6-2-1-3-7(4-6)12-5-13/h1-4H
InchiKey:	GFEPANUKFYVALF-UHFFFAOYSA-N
Formula:	C8H4F3NS
SMILES:	FC(F)(F)c1cccc(N=C=S)c1
Mol. weight [g/mol]:	203.18
CAS:	1840-19-3

Physical Properties

Property code	Value	Unit	Source
hf	-296.40	kJ/mol	Joback Method
hvap	43.03	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.440		Crippen Method
mcvol	122.860	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	554.63	K	Joback Method
tc	791.81	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1840193&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tc:	Critical Temperature