Benzene, 1-isocyanato-2-(trifluoromethyl)-

Other names:	Isocyanic acid, «alpha»,«alpha»,«alpha»-trifluoro-o-tolyl ester o-(Trifluoromethyl)phenyl isocyanate 2-(Trifluoromethyl)phenyl isocyanate «alpha»,«alpha»,«alpha»-Trifluoro-o-tolyl isocyanate 2-Trifluoromethylphenylaisocyanate
Inchi:	InChI=1S/C8H4F3NO/c9-8(10,11)6-3-1-2-4-7(6)12-5-13/h1-4H
InchiKey:	GZWGTVZRRFPVAS-UHFFFAOYSA-N
Formula:	C8H4F3NO
SMILES:	O=C=Nc1ccccc1C(F)(F)F
Mol. weight [g/mol]:	187.12
CAS:	2285-12-3

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	348.00	K	5.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2285123&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

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