1-(TRIFLUOROACETYL)IMIDAZOLE

Other names:	1-(Trifluoroacetyl)imidazole
	1H-Imidazole, 1-(trifluoroacetyl)-
	1-(trifluoroacetyl)-1H-imidazole
Inchi:	InChI=1S/C5H3F3N2O/c6-5(7,8)4(11)10-2-1-9-3-10/h1-3H
InchiKey:	SINBGNJPYWNUQI-UHFFFAOYSA-N
Formula:	C5H3F3N2O
SMILES:	O=C(n1ccnc1)C(F)(F)F
Mol. weight [g/mol]:	164.09

Physical Properties

Property code	Value	Unit	Source
ie	9.91	eV	NIST Webbook
logp	1.086		Crippen Method
mcvol	88.690	ml/mol	McGowan Method
rinpol	830.00		NIST Webbook
rinpol	830.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.00	K	5.10	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1546798&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure