

1H-Imidazole, 1-(2,2,3,3,3-pentafluoro-1-oxopropyl)-

Other names:	N-Pentafluoropropionylimidazole 2,2,3,3,3-Pentafluoro-1-(1H-imidazol-1-yl)propan-1-one 1-(2,2,3,3,3-pentafluoro-1-oxopropyl)-1H-imidazole
Inchi:	InChI=1S/C6H3F5N2O/c7-5(8,6(9,10)11)4(14)13-2-1-12-3-13/h1-3H
InchiKey:	VZUSRIIEPFQBNE-UHFFFAOYSA-N
Formula:	C6H3F5N2O
SMILES:	O=C(n1ccnc1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	214.09
CAS:	71735-32-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	1.721		Crippen Method
mcvol	106.320	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71735325&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/60-519-9/1H-Imidazole-1-2-2-3-3-3-pentafluoro-1-oxopropyl.pdf>

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