1H-Imidazole, 1-(pentafluorobenzoyl)-

Other names:	N-Pentafluorobenzoylimidazole
	1-pentafluorobenzoyl-1H-imidazole
Inchi:	InChI=1S/C10H3F5N2O/c11-5-4(10(18)17-2-1-16-3-17)6(12)8(14)9(15)7(5)13/h1-3H
InchiKey:	DOLREFXBQXCDOR-UHFFFAOYSA-N
Formula:	C10H3F5N2O
SMILES:	O=C(c1c(F)c(F)c(F)c(F)c1F)n1ccnc1
Mol. weight [g/mol]:	262.14
CAS:	75641-06-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	2.267		Crippen Method
mcvol	138.920	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75641064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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