n-Heptafluorobutyrylimidazole

Other names:	Heptafluorobutyrylimidazole
	1-Heptafluorobutyrylimidazole
	N-(Heptafluoro-n-butyryl)imidazole
	1H-Imidazole, 1-(2,2,3,3,4,4,4-heptafluoro-1-oxobutyl)-
	1-(2,2,3,3,4,4,4-heptafluoro-1-oxobutyl)-1H-imidazole
Inchi:	InChI=1S/C7H3F7N2O/c8-5(9,6(10,11)7(12,13)14)4(17)16-2-1-15-3-16/h1-3H
InchiKey:	MSYHGYDAVLDKCE-UHFFFAOYSA-N
Formula:	C7H3F7N2O
SMILES:	O=C(n1ccnc1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	264.10
CAS:	32477-35-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	2.356		Crippen Method
mcvol	123.950	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	330.00 ± 1.00	K	1.60	NIST Webbook

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=C32477353&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure