

L-proline, n-heptafluorobutyl-, decyl ester

Inchi:	InChI=1S/C19H28F7NO3/c1-2-3-4-5-6-7-8-9-13-30-15(28)14-11-10-12-27(14)16(29)17(2
InchiKey:	RBWZUOAVMQQOAD-UHFFFAOYSA-N
Formula:	C19H28F7NO3
SMILES:	CCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	451.42

Physical Properties

Property code	Value	Unit	Source
logp	5.494		Crippen Method
mcvol	299.090	ml/mol	McGowan Method
rinpol	2073.00		NIST Webbook
rinpol	2073.00		NIST Webbook
tb	595.06	K	Cheméo Relay (1.0)

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=U321104&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/40-346-3/L-proline-n-heptafluorobutyryl-decyl-ester.pdf>

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