L-Proline, N-heptafluorobutyryl-, octyl ester

Inchi: InChI=1S/C17H24F7NO3/c1-2-3-4-5-6-7-11-28-13(26)12-9-8-10-25(12)14(27)15(18,19)1
InchiKey: MQGCCDKQWWYMGS-UHFFFAOYSA-N
Formula: C17H24F7NO3
SMILES: CCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 423.37

Physical Properties

Property code	Value	Unit	Source
logp	4.714		Crippen Method
mcvol	270.910	ml/mol	McGowan Method
tb	572.74	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321103&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature