5-(4-Chlorophenyl)-6-ethylpyrimidine-2,4-diamine, N,N'-bis(pentafluoropropionyl)-

Inchi: InChI=1S/C18H11ClF10N4O2/c1-2-9-10(13-5-8(19)6-4-7)11(31-12(34)15(20,21)17(24,2

InchiKey: NNNZMLSRGFGSGS-UHFFFAOYSA-N

Formula: C18H11ClF10N4O2

SMILES: CCc1nc(NC(=O)C(F)(F)C(F)(F)F)nc(NC(=O)C(F)(F)C(F)(F)F)c1-c1ccc(Cl)cc1

Mol. weight [g/mol]: 540.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.29		Crippen Method
logp	5.632		Crippen Method
mcvol	289.960	ml/mol	McGowan Method
rinpol	2072.00		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=U373243&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices