

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

InChI: ClC1=CC=C(C=C1)C2=NC(=O)C(F)(F)C(F)(F)Fnc2C(F)(F)C(F)(F)FNC(=O)C(F)(F)C(F)(F)F
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/ci9903071>
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

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