

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

InChI: CCc1nc(NC(=O)C(F)(F)F)nc(NC(=O)C(F)(F)F)c1-c1ccc(Cl)cc1
InChIKey: RDRARQKIKYLSPL-UHF7FAOYSA-N
Formula: C₁₆H₁₁ClF₆N₄O₂
SMILES: CCc1nc(NC(=O)C(F)(F)F)nc(NC(=O)C(F)(F)F)c1-c1ccc(Cl)cc1
Mol. weight [g/mol]: 440.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	4.361		Crippen Method
mcvol	254.700	ml/mol	McGowan Method
rinpol	2150.00		NIST Webbook

Sources

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=U373242&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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