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

**Inchi:** InChI=1S/C20H11ClF14N4O2/c1-2[illegible]10(7-3-5-8(21)6-4-7)11(37-12(40)15(22,23)17(26,2

**InchiKey:** PDRDWYIUWFOWEG-UHFFAOYSA-N

**Formula:** C20H11ClF14N4O2

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

**Mol. weight [g/mol]:** 640.76

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -9.75 | | Crippen Method |
| logp | 6.902 | | Crippen Method |
| mcvol | 325.220 | ml/mol | McGowan Method |
| rinpol | 2135.00 | | NIST Webbook |
| rinpol | 2135.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U373253&Units=SI

**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

## 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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