

(5-Chloro-2-nitrophenyl)methanol, dimethylpentafluorophenylsilyl ether

Inchi: InChI=1S/C15H11ClF5NO3Si/c1-26(2,15-13(20)11(18)10(17)12(19)14(15)21)25-6-7-5-8
InchiKey: QFBVAIOFAYFHOS-UHFFFAOYSA-N
Formula: C15H11ClF5NO3Si
SMILES: C[Si](C)(OCc1cc(Cl)ccc1[N+](=O)[O-])c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 411.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.91		Crippen Method
logp	4.573		Crippen Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368735&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/64-184-7/5-Chloro-2-nitrophenyl-methanol-dimethylpentafluorophenylsilyl-ether.pdf>

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