

# 6-Chloro-N-sec-butyl-N'-heptafluorobutryl-1,3,5-triazine-2,4-diamine

<b>Other names:</b>	N-sec-Butyl-N'-butryl-6-chloro-1,3,5-triazine-2,4-diamine
<b>Inchi:</b>	InChI=1S/C11H11ClF7N5O/c1-3-4(2)20-7-22-6(12)23-8(24-7)21-5(25)9(13,14)10(15,16)
<b>InchiKey:</b>	MMNUBPSZBLIDOK-UHFFFAOYSA-N
<b>Formula:</b>	C11H11ClF7N5O
<b>SMILES:</b>	CCC(C)Nc1nc(Cl)nc(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)n1
<b>Mol. weight [g/mol]:</b>	397.68

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	3.507		Crippen Method
mcvol	218.190	ml/mol	McGowan Method
rinpol	1684.00		NIST Webbook
rinpol	1684.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U372981&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U372981&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/53-985-0/6-Chloro-N-sec-butyl-N-heptafluorobutryl-1-3-5-triazine-2-4-diamine.pdf>

Generated by Cheméo on 2024-04-26 15:05:05.574515021 +0000 UTC m=+16433154.495092337.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.