

s-Triazine, 2-chloro-4-(isopropylamino)-6-(methylamino)-

Other names:	2-Chloro-4-isopropylamino-6-methylamino-s-triazine G-30,026 GEIGY 30026 2-Methylamino-4-isopropylamino-6-chloro-s-triazine Norazine
Inchi:	InChI=1S/C7H12ClN5/c1-4(2)10-7-12-5(8)11-6(9-3)13-7/h4H,1-3H3,(H2,9,10,11,12,13)
InchiKey:	KLJYRZOFJHYOCO-UHFFFAOYSA-N
Formula:	C7H12ClN5
SMILES:	CNc1nc(Cl)nc(NC(C)C)n1
Mol. weight [g/mol]:	201.66
CAS:	3004-71-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	1.387		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
ripol	2761.00		NIST Webbook
ripol	2761.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3004715&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

ripol: Polar retention indices

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