2-1-methylbutylamino-4,6-dichloro-s-triazine

Inchi: InChI=1S/C8H12Cl2N4/c1-3-4-5(2)11-8-13-6(9)12-7(10)14-8/h5H,3-4H2,1-2H3,(H,11,12,
InchiKey: RBJAOUBQAQYPIF-UHFFFAOYSA-N
Formula: C8H12Cl2N4
SMILES: CCCC(C)Nc1nc(Cl)nc(Cl)n1
Mol. weight [g/mol]: 235.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.18		Cheméo Relay (1.0)
logp	2.779		Crippen Method
mcvol	164.220	ml/mol	McGowan Method
rinpol	1653.61		NIST Webbook
rinpol	1670.78		NIST Webbook
rinpol	1668.31		NIST Webbook
rinpol	1678.79		NIST Webbook
rinpol	1643.16		NIST Webbook
rinpol	1668.31		NIST Webbook
rinpol	1643.16		NIST Webbook
rinpol	1643.16		NIST Webbook
rinpol	1668.31		NIST Webbook
tf	351.45	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R288563&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point