2,4-bis(1,3-dimethylbutyl-amino)-6-chloro-s-triazi

Inchi: InChI=1S/C15H28ClN5/c1-9(2)7-11(5)17-14-19-13(16)20-15(21-14)18-12(6)8-10(3)4/h9-
InchiKey: HSYFFQOHBSEBHZ-UHFFFAOYSA-N
Formula: C15H28ClN5
SMILES: CC(C)CC(C)Nc1nc(Cl)nc(NC(C)CC(C)C)n1
Mol. weight [g/mol]: 313.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.98		Cheméo Relay (1.0)
logp	4.218		Crippen Method
mcvol	260.590	ml/mol	McGowan Method
rinpol	2123.87		NIST Webbook
rinpol	2123.87		NIST Webbook
rinpol	2188.26		NIST Webbook
rinpol	2188.26		NIST Webbook
rinpol	2138.81		NIST Webbook
rinpol	2151.76		NIST Webbook
rinpol	2188.26		NIST Webbook
rinpol	2203.23		NIST Webbook
rinpol	2123.87		NIST Webbook
tf	390.05	K	Cheméo Relay (1.0)

Sources

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=R288647&Units=SI
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
tf:	Normal melting (fusion) point