CHLORPROGUANIL

Other names: Chlorproguanil
1-(3,4-Dichlorophenyl)-5-isopropylbiguanide
M-5943
Inchi: InChI=1S/C11H15Cl2N5/c1-6(2)16-10(14)18-11(15)17-7-3-4-8(12)9(13)5-7/h3-6H,1-2H3
InchiKey: ISZNZKHCRKXXAU-UHFFFAOYSA-N
Formula: C11H15Cl2N5
SMILES: CC(C)NC(=N)NC(=N)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 288.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.86		Cheméo Relay (1.0)
logp	2.862		Crippen Method
mcvol	207.870	ml/mol	McGowan Method
rinpol	1621.00		NIST Webbook
rinpol	1621.00		NIST Webbook
tf	453.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.62	J/mol×K	881.33	Joback Method
cpg	88.02	J/mol×K	100.12	Joback Method
cpg	88.02	J/mol×K	100.12	Joback Method
cpg	88.02	J/mol×K	100.12	Joback Method
cpg	88.02	J/mol×K	100.12	Joback Method
cpg	88.02	J/mol×K	100.12	Joback Method
cpg	88.02	J/mol×K	100.12	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C537213&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

cpg:	Ideal gas heat capacity
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