

2-chloro-N,N,6-trimethylpyrimidin-4-amine

Inchi:	InChI=1S/C7H10ClN3/c1-5-4-6(11(2)3)10-7(8)9-5/h4H,1-3H3
InchiKey:	HJIUPFPIEBPYIE-UHFFFAOYSA-N
Formula:	C7H10ClN3
SMILES:	<chem>Cc1cc(N(C)C)nc(Cl)n1</chem>
Mol. weight [g/mol]:	171.63
CAS:	535-89-7

Physical Properties

Property code	Value	Unit	Source
af	0.4652		Cheméo Relay (1.0)
hvap	67.11	kJ/mol	Cheméo Relay (1.0)
ie	8.39	eV	Cheméo Relay (1.0)
logp	1.504		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
pc	3525.03	kPa	Cheméo Relay (1.0, beta)
tb	519.16	K	Cheméo Relay (1.0)
tc	737.76	K	Cheméo Relay (1.0)
tf	360.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
McGowan Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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