Piperazine, 1-[(4-chlorophenyl)phenylmethyl]-

Other names: Piperazine, 1-[(4-chlorophenyl)phenylmethyl]-
N-(p-Chlorobenzhydryl)piperazine
1-(4-Chlorobenzhydryl)piperazine
4-(4-Chlorobenzhydryl)piperazine
1-(4-Chloro-«alpha»-phenylbenzyl)piperazine
1-(«alpha»-Phenyl-4-chlorobenzyl)piperazine
Piperazine, 1-(p-chloro-«alpha»-phenylbenzyl)-
Piperazine, 1-(«alpha»-(4-chlorophenyl)benzyl)-
1-[(4-Chlorophenyl)(phenyl)methyl]piperazine
N-(4-Chlorobenzhydryl)piperazine
NSC 86164

Inchi: InChI=1S/C17H19ClN2/c18-16-8-6-15(7-9-16)17(14-4-2-1-3-5-14)20-12-10-19-11-13-20/

InchiKey: UZKBSZSTDQSMDR-UHFFFAOYSA-N

Formula: C17H19ClN2

SMILES: Clc1ccc(C(c2ccccc2)N2CCNCC2)cc1

Mol. weight [g/mol]: 286.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Cheméo Relay (1.0)
logp	3.335		Crippen Method
mcvol	224.210	ml/mol	McGowan Method
tb	658.27	K	Cheméo Relay (1.0)
tf	356.30	K	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	452.20	K	0.07	NIST Webbook

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C303264&Units=SI
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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point