Pentanamide, N-(4-chlorophenyl)-2,2-dimethyl-

Other names:	Pentanamide, N-(4-chlorophenyl)-2,2-dimethyl-
	Valeranilide, 4'-chloro-2,2-dimethyl-
	D 90A
	N-(4-Chlorophenyl)-«alpha»,«alpha»-Dimethylvaleramide
	Potablan
	4-Chloranilid kyseliny 2,2-dimethylvalerove
	N-(4-Chlorophenyl)-2,2-dimethylpentanamide
	N-(4-Chlorophenyl)-2,2-dimethylvaleroamide
	N-(4-Chlorphenyl)-2,2-dimethylpentamid
	N-(4-Chlor-phenyl)-2,2-dimethyl-valeriansaeureamid
	Schering-35830
	SN 35830
Inchi:	InChI=1S/C13H18ClNO/c1-4-9-13(2,3)12(16)15-11-7-5-10(14)6-8-11/h5-8H,4,9H2,1-3H3
InchiKey:	KXGYBSNVFXBPNO-UHFFFAOYSA-N
Formula:	C13H18ClNO
SMILES:	CCCC(C)(C)C(=O)Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	239.75

Physical Properties

Property code	Value	Unit	Source
hfus	26.56	kJ/mol	Joback Method
ie	8.15	eV	Cheméo Relay (1.0)
log10ws	-4.39		Cheméo Relay (1.0)
logp	4.105		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
tf	371.31	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.82	J/mol×K	666.74	Joback Method
cpg	515.86	J/mol×K	703.56	Joback Method
cpg	529.85	J/mol×K	740.38	Joback Method
cpg	542.83	J/mol×K	777.20	Joback Method

cpg	554.89	J/mol×K	814.02	Joback Method
cpg	566.10	J/mol×K	850.84	Joback Method
cpg	576.51	J/mol×K	887.67	Joback Method

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?Str2File=C7287367
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point