Pentanamide, N-(3-chloro-4-methylphenyl)-2-methyl-

Other names: p-Valerotoluidide, 3'-chloro-2-methyl-
Chlorpentan
CMA
CMMP
Dutom
Hortox
Niagara 4512
Pentanochlor
Solan
Solan (Herbicide)
Solane
N-(3-Chlor-methylphenyl)-2-methylpentanamid
N-(3-Chloro-4-methylphenyl)-2-methylpentanamide
3'-Chloro-2-methyl-p-valerotoluidide
Dakuron
FMC 4512
Pentachlore
(3-Chloro-4-(methylphenyl))-2-methylpentamide
Pentanochlore

Inchi: InChI=1S/C13H18ClNO/c1-4-5-10(3)13(16)15-11-7-6-9(2)12(14)8-11/h6-8,10H,4-5H2,1-3

InchiKey: WGVWLKXZBUVUAM-UHFFFAOYSA-N

Formula: C13H18ClNO

SMILES: CCCC(C)C(=O)Nc1ccc(C)c(Cl)c1

Mol. weight [g/mol]: 239.74

CAS: 2307-68-8

Physical Properties

Property code	Value	Unit	Source
gf	97.83	kJ/mol	Joback Method
hf	-178.19	kJ/mol	Joback Method
hfus	30.06	kJ/mol	Joback Method
hvap	65.31	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	4.023		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
tb	674.51	K	Joback Method

tc	888.72	K	Joback Method
tf	355.94 ± 0.20	K	NIST Webbook
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.52	J/mol×K	674.51	Joback Method
cpg	512.15	J/mol×K	710.21	Joback Method
cpg	525.86	J/mol×K	745.91	Joback Method
cpg	538.69	J/mol×K	781.62	Joback Method
cpg	550.68	J/mol×K	817.32	Joback Method
cpg	561.86	J/mol×K	853.02	Joback Method
cpg	572.27	J/mol×K	888.72	Joback Method
hfust	16.35	kJ/mol	353.20	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2307688&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume