Monalide

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]:	239.74
CAS:	7287-36-7

Physical Properties

Property code	Value	Unit	Source
gf	112.74	kJ/mol	Joback Method
hf	-170.19	kJ/mol	Joback Method
hfus	26.56	kJ/mol	Joback Method
hvap	63.74	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	4.105		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
tb	666.74	K	Joback Method
tc	887.67	K	Joback Method
tf	360.65 ± 0.20	K	NIST Webbook
vc	0.735	m3/kmol	Joback Method

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
hfust	23.31	kJ/mol	360.20	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7287367&Units=SI

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