L-Leucyl-p-nitroanilide

Other names:	L-Leucine-p-nitroanilide
	L-Leucine-p-nitroaniline
	L-Leucine-4-nitroanilide
	Pentanamide, 2-amino-4-methyl-N-(4-nitrophenyl)-, (S)-
	(S)-2-amino-4-methyl-N-(4-nitrophenyl)valeramide
Inchi:	InChI=1S/C12H17N3O3/c1-8(2)7-11(13)12(16)14-9-3-5-10(6-4-9)15(17)18/h3-6,8,11H,7,
InchiKey:	AXZJHDNQDSVIDR-LLVKDONJSA-N
Formula:	C12H17N3O3
SMILES:	CC(C)CC(N)C(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	251.28
CAS:	4178-93-2

Physical Properties

Property code	Value	Unit	Source
gf	210.53	kJ/mol	Joback Method
hf	-112.59	kJ/mol	Joback Method
hfus	36.70	kJ/mol	Joback Method
hvap	84.88	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	1.907		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
tb	833.15	K	Joback Method
tc	1075.73	K	Joback Method
tf	563.40	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.22	J/mol×K	833.15	Joback Method
cpg	594.42	J/mol×K	873.58	Joback Method
cpg	605.56	J/mol×K	914.01	Joback Method
cpg	615.71	J/mol×K	954.44	Joback Method

cpg	624.93	J/mol×K	994.87	Joback Method
cpg	633.30	J/mol×K	1035.30	Joback Method
cpg	640.87	J/mol×K	1075.73	Joback Method

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=C4178932&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
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