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-UHFFFAOYSA-N
Formula:	C12H17N3O3
SMILES:	CC(C)CC(N)C(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	251.29

Physical Properties

Property code	Value	Unit	Source
hfus	36.70	kJ/mol	Joback Method
ie	8.31	eV	Cheméo Relay (1.0)
log10ws	-3.35		Cheméo Relay (1.0)
logp	1.907		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
tf	452.49	K	Cheméo Relay (1.0)

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

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4178932&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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