

Valeramide, 5-chloro-N-pentyl-

Inchi: InChI=1S/C10H20ClNO/c1-2-3-6-9-12-10(13)7-4-5-8-11/h2-9H2,1H3,(H,12,13)
InchiKey: NXTVLYPQRFOPMW-UHFFFAOYSA-N
Formula: C10H20ClNO
SMILES: CCCCCN=C(O)CCCCCl
Mol. weight [g/mol]: 205.72

Physical Properties

Property code	Value	Unit	Source
hf	-345.27	kJ/mol	Joback Method
hvap	62.31	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.542		Crippen Method
mcvol	175.550	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1724.00		NIST Webbook
tb	634.37	K	Joback Method
tc	814.73	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407533&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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