

Valeramide, 5-chloro-N-(hept-2-yl)-

Inchi:	InChI=1S/C12H24ClNO/c1-3-4-5-8-11(2)14-12(15)9-6-7-10-13/h11H,3-10H2,1-2H3,(H,14)
InchiKey:	GVVUQONPDQIHEP-UHFFFAOYSA-N
Formula:	C12H24ClNO
SMILES:	CCCCC(C)N=C(O)CCCCI
Mol. weight [g/mol]:	233.78

Physical Properties

Property code	Value	Unit	Source
hf	-391.83	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	4.321		Crippen Method
mcpvol	203.730	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	1802.00		NIST Webbook
rinpol	1802.00		NIST Webbook
tb	679.69	K	Joback Method
tc	860.79	K	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=U407534&Units=SI

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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