

Valeramide, N-hexyl-

Other names:	Pentanamide, N-hexyl
Inchi:	InChI=1S/C11H23NO/c1-3-5-7-8-10-12-11(13)9-6-4-2/h3-10H2,1-2H3,(H,12,13)
InchiKey:	HYTMILDAGQOHDF-UHFFFAOYSA-N
Formula:	C11H23NO
SMILES:	CCCCCN=C(O)CCCC
Mol. weight [g/mol]:	185.31
CAS:	10264-25-2

Physical Properties

Property code	Value	Unit	Source
hf	-350.17	kJ/mol	Joback Method
hvap	60.15	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.713		Crippen Method
mcvol	177.400	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1516.00		NIST Webbook
tb	619.82	K	Joback Method
tc	794.62	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10264252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/82-813-8/Valeramide-N-hexyl.pdf>

Generated by Cheméo on 2024-04-29 01:56:25.140318024 +0000 UTC m=+16645034.060895336.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.