

Phenylacetamide, N-heptyl-

Inchi:	InChI=1S/C15H23NO/c1-2-3-4-5-9-12-16-15(17)13-14-10-7-6-8-11-14/h6-8,10-11H,2-5,9
InchiKey:	ISTRCHUUBRFZEZ-UHFFFAOYSA-N
Formula:	C15H23NO
SMILES:	CCCCCCCN=C(O)Cc1ccccc1
Mol. weight [g/mol]:	233.35

Physical Properties

Property code	Value	Unit	Source
hf	-196.20	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.156		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinsol	2002.00		NIST Webbook
tb	738.02	K	Joback Method
tc	936.48	K	Joback Method

Sources

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=U407228&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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