

Phenylacetamide, N-(hept-2-yl)-

Inchi: InChI=1S/C15H23NO/c1-3-4-6-9-13(2)16-15(17)12-14-10-7-5-8-11-14/h5,7-8,10-11,13H,
InchiKey: AXQPRWQTJNNBAO-UHFFFAOYSA-N
Formula: C15H23NO
SMILES: CCCCCC(C)N=C(O)Cc1ccccc1
Mol. weight [g/mol]: 233.35

Physical Properties

Property code	Value	Unit	Source
hf	-201.48	kJ/mol	Joback Method
hvap	70.94	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.154		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1863.00		NIST Webbook
rinpol	1863.00		NIST Webbook
tb	737.58	K	Joback Method
tc	938.94	K	Joback Method

Sources

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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407225&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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