Phenylacetamide, N-octyl-

Inchi: InChI=1S/C16H25NO/c1-2-3-4-5-6-10-13-17-16(18)14-15-11-8-7-9-12-15/h7-9,11-12H,2-
InchiKey: AKPIJQRYVLUWRL-UHFFFAOYSA-N
Formula: C16H25NO
SMILES: CCCCCCCCN=C(O)Cc1ccccc1
Mol. weight [g/mol]: 247.38

Physical Properties

Property code	Value	Unit	Source
hf	-216.84	kJ/mol	Joback Method
hvap	73.56	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.546		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	2109.00		NIST Webbook
rinpol	2109.00		NIST Webbook
tb	760.90	K	Joback Method
tc	958.16	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=U407229&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