

Phenylacetamide, N-tetradecyl-

Inchi: InChI=1S/C22H37NO/c1-2-3-4-5-6-7-8-9-10-11-12-16-19-23-22(24)20-21-17-14-13-15-16
InchiKey: FQMQTIRWQFVVLS-UHFFFAOYSA-N
Formula: C22H37NO
SMILES: CCCCCCCCCCCCCCN=C(O)Cc1ccccc1
Mol. weight [g/mol]: 331.54

Physical Properties

Property code	Value	Unit	Source
hf	-340.68	kJ/mol	Joback Method
hvap	86.91	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	6.887		Crippen Method
mcvol	308.630	ml/mol	McGowan Method
pc	1105.94	kPa	Joback Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook
tb	898.18	K	Joback Method
tc	1101.49	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=U407234&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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