

p-Hexyloxybenzylidene p-octylaniline

Inchi: InChI=1S/C27H39NO/c1-3-5-7-9-10-11-13-24-14-18-26(19-15-24)28-23-25-16-20-27(21-22)
InchiKey: ZIEZBSKSIITGJE-UHFFFAOYSA-N
Formula: C27H39NO
SMILES: CCCCCCCc1ccc(N=Cc2ccc(OCCCCC)cc2)cc1
Mol. weight [g/mol]: 393.60
CAS: 39777-28-1

Physical Properties

Property code	Value	Unit	Source
hf	-200.49	kJ/mol	Joback Method
hvap	87.30	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	8.299		Crippen Method
mcvol	355.320	ml/mol	McGowan Method
pc	918.27	kPa	Joback Method
tb	979.58	K	Joback Method
tc	1202.89	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=C39777281&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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