

p-bromobenzylidene-hexyl-amine

Inchi: InChI=1S/C13H18BrN/c1-2-3-4-5-10-15-11-12-6-8-13(14)9-7-12/h6-9,11H,2-5,10H2,1H3
InchiKey: NGYANEKCNAAEAMK-RVDMUPIBSA-N
Formula: C13H18BrN
SMILES: CCCCCCN=Cc1ccc(Br)cc1
Mol. weight [g/mol]: 268.19

Physical Properties

Property code	Value	Unit	Source
hf	21.96	kJ/mol	Joback Method
hvap	57.22	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.448		Crippen Method
mcvol	193.450	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1884.00		NIST Webbook
tb	671.34	K	Joback Method
tc	896.57	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R159663&Units=SI>
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>

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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