

p-methoxybenzylidene-butyl-amine

Inchi: InChI=1S/C12H17NO/c1-3-4-9-13-10-11-5-7-12(14-2)8-6-11/h5-8,10H,3-4,9H2,1-2H3/b1
InchiKey: RYTXIPUXGFCMPB-JLHYYAGUSA-N
Formula: C12H17NO
SMILES: CCCCN=Cc1ccc(OC)cc1
Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
hf	-115.95	kJ/mol	Joback Method
hvap	50.97	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.914		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
tb	604.72	K	Joback Method
tc	819.58	K	Joback Method

Sources

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=R160099&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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