

(p-methylbenzylidene)-butyl-amine

Inchi:	InChI=1S/C12H17N/c1-3-4-9-13-10-12-7-5-11(2)6-8-12/h5-8,10H,3-4,9H2,1-2H3
InchiKey:	NSSZZXRKKBIESQ-UHFFFAOYSA-N
Formula:	C12H17N
SMILES:	CCCCN=Cc1ccc(C)cc1
Mol. weight [g/mol]:	175.27

Physical Properties

Property code	Value	Unit	Source
hf	16.27	kJ/mol	Joback Method
hvap	48.56	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.214		Crippen Method
mcpvol	161.860	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1479.00		NIST Webbook
rinpol	1479.00		NIST Webbook
tb	582.30	K	Joback Method
tc	799.73	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R160331&Units=SI
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

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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