

(Z)-N-methoxy-1-(4-methylphenyl)propanimine

Inchi: InChI=1S/C12H17NO/c1-4-5-12(13-14-3)11-8-6-10(2)7-9-11/h6-9H,4-5H2,1-3H3
InchiKey: ZNADZQURDYANQD-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CCCC(=NOC)c1ccc(C)cc1
Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
hf	-125.74	kJ/mol	Joback Method
hvap	51.05	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.146		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1391.00		NIST Webbook
rinpol	1391.00		NIST Webbook
tb	604.60	K	Joback Method
tc	823.22	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=U373233&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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