

N-vanillylidene aniline

Inchi:	InChI=1S/C14H13NO2/c1-17-14-9-11(7-8-13(14)16)10-15-12-5-3-2-4-6-12/h2-10,16H,1H
InchiKey:	NQTPEBUGIFUYEC-XNTDXEJSSA-N
Formula:	C14H13NO2
SMILES:	COc1cc(C=Nc2ccccc2)ccc1O
Mol. weight [g/mol]:	227.26
CAS:	17696-53-6

Physical Properties

Property code	Value	Unit	Source
hf	-98.01	kJ/mol	Joback Method
hvap	70.71	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	3.151		Crippen Method
mcvol	178.020	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
tb	757.78	K	Joback Method
tc	1016.01	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17696536&Units=SI

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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