

Noxiptyline M(Nor-HO), acetylated

Inchi: InChI=1S/C22H24N2O4/c1-15(25)24(3)12-13-27-23-22-20-7-5-4-6-17(20)8-9-18-14-19(2)
InchiKey: UBNVSMLETHYHCIB-UHFFFAOYSA-N
Formula: C22H24N2O4
SMILES: CC(=O)Oc1ccc2c(c1)CCc1cccc1C2=NOCCN(C)C(C)=O
Mol. weight [g/mol]: 380.44

Physical Properties

Property code	Value	Unit	Source
hf	-346.66	kJ/mol	Joback Method
hvap	95.82	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	2.958		Crippen Method
mcvol	293.000	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinsol	2750.00		NIST Webbook
tb	1026.65	K	Joback Method
tc	1268.72	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=R311163&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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