Noxiptyline M(Nor-di-HO), diacetylated

Inchi: InChI=1S/C24H26N2O6/c1-15(27)26(4)11-12-30-25-24-22-9-7-20(31-16(2)28)13-18(22)5
InchiKey: ZZCKVKJZGIBALP-UHFFFAOYSA-N
Formula: C24H26N2O6
SMILES: CC(=O)Oc1ccc2c(c1)CCc1cc(OC(C)=O)ccc1C2=NOCCN(C)C(C)=O
Mol. weight [g/mol]: 438.47

Physical Properties

Property code	Value	Unit	Source
hf	-644.21	kJ/mol	Joback Method
hvap	110.09	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	2.883		Crippen Method
mcvol	328.620	ml/mol	McGowan Method
pc	1323.28	kPa	Joback Method
rinpol	3020.00		NIST Webbook
tb	1153.68	K	Joback Method
tc	1412.69	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=R311158&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

Latest version available from:
https://www.chemeo.com/cid/10-610-2/Noxiptyline-M-Nor-di-HO-diacetylated.pdf
Generated by Cheméo on 2024-04-25 17:42:39.612075015 +0000 UTC m=+16356208.532652330.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.