5-(3-Acetamidopropyl)-5H-dibenzo[a,d]cyclohepte

Other names: Protriptyline M(Nor), acetylated
Inchi: InChI=1S/C20H21NO/c1-15(22)21-14-6-11-20-18-9-4-2-7-16(18)12-13-17-8-3-5-10-19(1
InchiKey: NCRPPNXANDRVKZ-UHFFFAOYSA-N
Formula: C20H21NO
SMILES: CC(O)=NCCCC1c2ccccc2C=Cc2ccccc21
Mol. weight [g/mol]: 291.39
CAS: 19070-26-9

Physical Properties

Property code	Value	Unit	Source
hf	44.77	kJ/mol	Joback Method
hvap	86.27	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	5.059		Crippen Method
mcvol	241.530	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tb	894.96	K	Joback Method
tc	1126.30	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=C19070269&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