Amitriptyline N-oxide M(Desoxo-nor-HO)

Inchi: InChI=1S/C19H19NO/c1-20-12-4-7-18-17-6-3-2-5-14(17)8-9-15-10-11-16(21)13-19(15)18
InchiKey: PTFFXHUUCUKLPG-WSVATBPTSA-N
Formula: C19H19NO
SMILES: CNCCC=C1c2ccccc2C=Cc2ccc(O)cc21
Mol. weight [g/mol]: 277.36

Physical Properties

Property code	Value	Unit	Source
gf	393.31	kJ/mol	Joback Method
hf	117.74	kJ/mol	Joback Method
hfus	41.76	kJ/mol	Joback Method
hvap	84.52	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.917		Crippen Method
mcvol	227.440	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	2670.00		NIST Webbook
tb	845.44	K	Joback Method
tc	1090.97	K	Joback Method
tf	579.45	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.04	J/mol×K	845.44	Joback Method
cpg	684.81	J/mol×K	886.36	Joback Method
cpg	699.02	J/mol×K	927.28	Joback Method
cpg	712.88	J/mol×K	968.20	Joback Method
cpg	726.59	J/mol×K	1009.13	Joback Method
cpg	740.35	J/mol×K	1050.05	Joback Method
cpg	754.37	J/mol×K	1090.97	Joback Method

Sources

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=R212992&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume