

Amitriptyline N-oxide M(Desoxo-HO)

Inchi:	InChI=1S/C20H21NO/c1-21(2)13-5-8-19-18-7-4-3-6-15(18)9-10-16-11-12-17(22)14-20(1)
InchiKey:	UHLPYBQGKLFHIFK-UWVJJOHFNSA-N
Formula:	C20H21NO
SMILES:	CN(C)CCC=C1c2ccccc2C=Cc2ccc(O)cc21
Mol. weight [g/mol]:	291.39

Physical Properties

Property code	Value	Unit	Source
gf	423.12	kJ/mol	Joback Method
hf	111.16	kJ/mol	Joback Method
hfus	42.27	kJ/mol	Joback Method
hvap	82.35	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.259		Crippen Method
mcvol	241.530	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	2236.00		NIST Webbook
tb	830.59	K	Joback Method
tc	1070.96	K	Joback Method
tf	570.53	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.21	J/molxK	830.59	Joback Method
cpg	728.94	J/molxK	870.65	Joback Method
cpg	744.01	J/molxK	910.71	Joback Method
cpg	758.63	J/molxK	950.77	Joback Method
cpg	772.99	J/molxK	990.84	Joback Method
cpg	787.31	J/molxK	1030.90	Joback Method
cpg	801.79	J/molxK	1070.96	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=R212987&Units=SI

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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