Hydroxynortriptyline

Inchi: InChI=1S/C19H21NO/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: DXTZQTSIXRYNQV-WSVATBPTSA-N
Formula: C19H21NO
SMILES: CNCCC=C1c2ccccc2CCc2ccc(O)cc21
Mol. weight [g/mol]: 279.38

Physical Properties

Property code	Value	Unit	Source
hfus	40.54	kJ/mol	Joback Method
ie	7.80	eV	Cheméo Relay (1.0)
log10ws	-3.46		Cheméo Relay (1.0)
logp	3.532		Crippen Method
mcvol	231.740	ml/mol	McGowan Method
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook
tf	456.87	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.31	J/mol×K	846.28	Joback Method
cpg	713.95	J/mol×K	886.90	Joback Method
cpg	728.96	J/mol×K	927.52	Joback Method
cpg	743.56	J/mol×K	968.14	Joback Method
cpg	757.92	J/mol×K	1008.76	Joback Method
cpg	772.25	J/mol×K	1049.38	Joback Method
cpg	786.74	J/mol×K	1090.00	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R21934&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point