

Amitriptyline M(HO)

Inchi:	InChI=1S/C20H23NO/c1-21(2)13-5-8-20-18-7-4-3-6-15(18)9-10-16-14-17(22)11-12-19(1
InchiKey:	ZKUFJLAUUTUSLH-ZBKNUEDVSA-N
Formula:	C20H23NO
SMILES:	CN(C)CCC=C1c2ccccc2CCc2cc(O)ccc21
Mol. weight [g/mol]:	293.40

Physical Properties

Property code	Value	Unit	Source
gf	393.16	kJ/mol	Joback Method
hf	53.38	kJ/mol	Joback Method
hfus	41.05	kJ/mol	Joback Method
hvap	82.06	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.874		Crippen Method
mcvol	245.830	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinqol	2236.00		NIST Webbook
tb	831.43	K	Joback Method
tc	1070.04	K	Joback Method
tf	569.77	K	Joback Method
vc	0.865	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.12	J/molxK	831.43	Joback Method
cpg	757.73	J/molxK	871.20	Joback Method
cpg	773.61	J/molxK	910.97	Joback Method
cpg	788.97	J/molxK	950.74	Joback Method
cpg	804.00	J/molxK	990.51	Joback Method
cpg	818.91	J/molxK	1030.27	Joback Method
cpg	833.89	J/molxK	1070.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R212947&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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