

Amitriptyline M(Nor-HO), acetylated

Inchi:	InChI=1S/C23H25NO3/c1-16(25)24(3)14-6-9-23-21-8-5-4-7-18(21)10-11-19-15-20(27-17
InchiKey:	QACZKVNMTAMMPC-NUGSKGIGSA-N
Formula:	C23H25NO3
SMILES:	CC(=O)Oc1ccc2c(c1)CCc1cccc1C2=CCCN(C)C(C)=O
Mol. weight [g/mol]:	363.45

Physical Properties

Property code	Value	Unit	Source
gf	200.57	kJ/mol	Joback Method
hf	-200.08	kJ/mol	Joback Method
hfus	47.03	kJ/mol	Joback Method
hvap	92.28	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.011		Crippen Method
mvol	291.240	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinpol	2670.00		NIST Webbook
tb	954.59	K	Joback Method
tc	1188.47	K	Joback Method
tf	626.47	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.49	J/molxK	954.59	Joback Method
cpg	931.10	J/molxK	993.57	Joback Method
cpg	944.77	J/molxK	1032.55	Joback Method
cpg	957.62	J/molxK	1071.53	Joback Method
cpg	969.78	J/molxK	1110.51	Joback Method
cpg	981.35	J/molxK	1149.49	Joback Method
cpg	992.45	J/molxK	1188.47	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=R310784&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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