

# Butriptyline

## Other names:

<b>Inchi:</b>	(±)-[10,11-dihydro-«beta»-methyl-5H-dibenzola,d]cycloheptene-5-propyl]di(methyl)ammonium chloride
<b>InchiKey:</b>	ALELTCQZDXAMQ-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>21</sub> H <sub>27</sub> N
<b>SMILES:</b>	CC(CC1c2ccccc2CCc2ccccc21)CN(C)C
<b>Mol. weight [g/mol]:</b>	293.45
<b>CAS:</b>	5585-73-9

## Physical Properties

Property code	Value	Unit	Source
gf	500.59	kJ/mol	Joback Method
hf	108.40	kJ/mol	Joback Method
hfus	35.08	kJ/mol	Joback Method
hvap	69.78	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.505		Crippen Method
mcvol	258.350	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2155.00		NIST Webbook
tb	761.94	K	Joback Method
tc	988.29	K	Joback Method
tf	439.72	K	Joback Method
vc	0.965	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.46	J/mol×K	761.94	Joback Method

cpg	791.50	J/mol×K	799.67	Joback Method
cpg	810.17	J/mol×K	837.39	Joback Method
cpg	827.60	J/mol×K	875.12	Joback Method
cpg	843.90	J/mol×K	912.84	Joback Method
cpg	859.19	J/mol×K	950.57	Joback Method
cpg	873.60	J/mol×K	988.29	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5585739&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5585739&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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