

# Protriptyline, N-acetyl-

<b>Other names:</b>	Protriptyline, acetylated
<b>Inchi:</b>	InChI=1S/C21H23NO/c1-16(23)22(2)15-7-12-21-19-10-5-3-8-17(19)13-14-18-9-4-6-11-2
<b>InchiKey:</b>	SKZTVWHSICONPY-UHFFFAOYSA-N
<b>Formula:</b>	C21H23NO
<b>SMILES:</b>	CC(=O)N(C)CCCC1c2ccccc2C=Cc2ccccc21
<b>Mol. weight [g/mol]:</b>	305.41
<b>CAS:</b>	23047-28-1

## Physical Properties

Property code	Value	Unit	Source
gf	404.07	kJ/mol	Joback Method
hf	58.88	kJ/mol	Joback Method
hfus	41.43	kJ/mol	Joback Method
hvap	77.21	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.561		Crippen Method
mcvol	255.620	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	2688.00		NIST Webbook
tb	815.41	K	Joback Method
tc	1045.12	K	Joback Method
tf	505.41	K	Joback Method
vc	0.963	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.62	J/molxK	815.41	Joback Method
cpg	780.44	J/molxK	853.69	Joback Method
cpg	796.09	J/molxK	891.98	Joback Method
cpg	810.71	J/molxK	930.26	Joback Method
cpg	824.42	J/molxK	968.55	Joback Method
cpg	837.35	J/molxK	1006.83	Joback Method
cpg	849.61	J/molxK	1045.12	Joback Method

# Sources

<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=C23047281&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23047281&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>rinpola:</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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