

Protriptyline M(HO), acetylated

Inchi:	InChI=1S/C23H25NO3/c1-16(25)24(3)14-6-9-22-21-8-5-4-7-18(21)10-11-19-12-13-20(15)
InchiKey:	GCFYTYXKKLCBHE-UHFFFAOYSA-N
Formula:	C23H25NO3
SMILES:	CC(=O)Oc1ccc2c(c1)C(CCCN(C)C(C)=O)c1ccccc1C=C2
Mol. weight [g/mol]:	363.45

Physical Properties

Property code	Value	Unit	Source
gf	177.36	kJ/mol	Joback Method
hf	-238.67	kJ/mol	Joback Method
hfus	49.00	kJ/mol	Joback Method
hvap	91.48	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.486		Crippen Method
mvol	291.240	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	2895.00		NIST Webbook
tb	942.44	K	Joback Method
tc	1173.24	K	Joback Method
tf	612.63	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.31	J/molxK	942.44	Joback Method
cpg	935.91	J/molxK	980.91	Joback Method
cpg	949.45	J/molxK	1019.37	Joback Method
cpg	962.03	J/molxK	1057.84	Joback Method
cpg	973.76	J/molxK	1096.31	Joback Method
cpg	984.76	J/molxK	1134.77	Joback Method
cpg	995.11	J/molxK	1173.24	Joback Method

Sources

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=R311198&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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