

Venlafaxine AC

Inchi: InChI=1S/C19H29NO3/c1-15(21)23-19(12-6-5-7-13-19)18(14-20(2)3)16-8-10-17(22-4)11
InchiKey: JGOQAINPLQITA-UHFFFAOYSA-N
Formula: C19H29NO3
SMILES: COc1ccc(C(CN(C)C)C2(OC(C)=O)CCCCC2)cc1
Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
gf	0.26	kJ/mol	Joback Method
hf	-455.64	kJ/mol	Joback Method
hfus	27.63	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.606		Crippen Method
mvol	267.240	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	796.28	K	Joback Method
tc	1018.33	K	Joback Method
tf	485.97	K	Joback Method
vc	0.977	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.06	J/molxK	796.28	Joback Method
cpg	852.62	J/molxK	833.29	Joback Method
cpg	872.20	J/molxK	870.30	Joback Method
cpg	890.92	J/molxK	907.30	Joback Method
cpg	908.93	J/molxK	944.31	Joback Method
cpg	926.36	J/molxK	981.32	Joback Method
cpg	943.34	J/molxK	1018.33	Joback Method

Sources

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=R331221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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