

Cyclohexanol, 1-[2-(dimethylamino)-1-(4-methoxyphenyl)ethyl]-

Other names:	Venlafaxine
Inchi:	InChI=1S/C17H27NO2/c1-18(2)13-16(17(19)11-5-4-6-12-17)14-7-9-15(20-3)10-8-14/h7-
InchiKey:	PNVNVHUZROJLTJ-UHFFFAOYSA-N
Formula:	C17H27NO2
SMILES:	COc1ccc(C(CN(C)C)C2(O)CCCCC2)cc1
Mol. weight [g/mol]:	277.40
CAS:	93413-69-5

Physical Properties

Property code	Value	Unit	Source
gf	80.52	kJ/mol	Joback Method
hf	-321.79	kJ/mol	Joback Method
hfus	23.75	kJ/mol	Joback Method
hvap	76.40	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.036		Crippen Method
mcvol	237.490	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	2133.10		NIST Webbook
rinpol	2133.10		NIST Webbook
tb	766.41	K	Joback Method
tc	977.73	K	Joback Method
tf	452.09	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.54	J/molxK	766.41	Joback Method
cpg	750.10	J/molxK	801.63	Joback Method
cpg	767.84	J/molxK	836.85	Joback Method
cpg	784.88	J/molxK	872.07	Joback Method
cpg	801.35	J/molxK	907.29	Joback Method
cpg	817.39	J/molxK	942.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C93413695&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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