

Viloxazine

Other names:	Morpholine, 2-[(2-ethoxyphenoxy)methyl]- 2-((2-Ethoxyphenoxy)methyl)morpholine 2-(2-Ethoxyphenoxy)methyl)tetrahydro-1,4-oxazine ICI-58834 Viloxazin 2-[(o-Ethoxyphenoxy)methyl]morpholine
Inchi:	InChI=1S/C13H19NO3/c1-2-15-12-5-3-4-6-13(12)17-10-11-9-14-7-8-16-11/h3-6,11,14H,1
InchiKey:	YWPHCCPCQOJSGZ-UHFFFAOYSA-N
Formula:	C13H19NO3
SMILES:	CCOc1cccc1OCC1CNCCO1
Mol. weight [g/mol]:	237.29
CAS:	46817-91-8

Physical Properties

Property code	Value	Unit	Source
gf	-22.60	kJ/mol	Joback Method
hf	-390.90	kJ/mol	Joback Method
hfus	34.86	kJ/mol	Joback Method
hvap	63.99	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.453		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	668.39	K	Joback Method
tc	898.88	K	Joback Method
tf	458.65	K	Joback Method
vc	0.682	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.50	J/mol×K	668.39	Joback Method

cpg	539.29	J/mol×K	706.80	Joback Method
cpg	556.82	J/mol×K	745.22	Joback Method
cpg	573.09	J/mol×K	783.63	Joback Method
cpg	588.10	J/mol×K	822.05	Joback Method
cpg	601.86	J/mol×K	860.46	Joback Method
cpg	614.36	J/mol×K	898.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C46817918&Units=SI
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

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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