

5-(3-Acetyl(methyl)aminopropylidene)-10-oxa-10,1

Other names:	Nordoxepin, acetylated
Inchi:	InChI=1S/C20H21NO2/c1-15(22)21(2)13-7-11-18-17-9-4-3-8-16(17)14-23-20-12-6-5-10-
InchiKey:	BFOHVUOMOVZBKO-WQRHYEAKSA-N
Formula:	C20H21NO2
SMILES:	CC(=O)N(C)CCC=C1c2ccccc2COc2ccccc21
Mol. weight [g/mol]:	307.39
CAS:	148324-75-8

Physical Properties

Property code	Value	Unit	Source
gf	332.74	kJ/mol	Joback Method
hf	-13.89	kJ/mol	Joback Method
hfus	44.85	kJ/mol	Joback Method
hvap	80.30	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.879		Crippen Method
mcvol	247.400	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	2700.00		NIST Webbook
rinpol	2700.00		NIST Webbook
tb	831.63	K	Joback Method
tc	1066.17	K	Joback Method
tf	534.55	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.55	J/molxK	831.63	Joback Method
cpg	749.02	J/molxK	870.72	Joback Method
cpg	763.48	J/molxK	909.81	Joback Method
cpg	777.05	J/molxK	948.90	Joback Method
cpg	789.87	J/molxK	987.99	Joback Method
cpg	802.07	J/molxK	1027.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C148324758&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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