Hordenine

Other names:	Phenol, 4-[2-(dimethylamino)ethyl]-
	Phenol, p-[2-(dimethylamino)ethyl]-
	p-[2-(Dimethylamino)ethyl]phenol
	p-Hydroxy-N,N-dimethylphenethylamine
	Anhalin
	Anhaline
	Eremursine
	Hordenin
	N,N-Dimethyl-p-hydroxyphenethylamine
	N,N-Dimethyltyramine
	Ordenina
	Ordenine
	Peyocactine
	N,N-Dimethyl-2-(4-hydroxyphenyl)ethylamine
	Cactine
	N,N-Dimethyl-4-hydroxy-«beta»-phenethylamine
	4-(2-dimethylaminoethyl)phenol
Inchi:	InChI=1S/C10H15NO/c1-11(2)8-7-9-3-5-10(12)6-4-9/h3-6,12H,7-8H2,1-2H3
InchiKey:	KUBCEEMXQZUPDQ-UHFFFAOYSA-N
Formula:	C10H15NO
SMILES:	CN(C)CCc1ccc(O)cc1
Mol. weight [g/mol]:	165.23
CAS:	539-15-1

Physical Properties

Property code	Value	Unit	Source
gf	101.89	kJ/mol	Joback Method
hf	-122.98	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hvap	55.19	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.496		Crippen Method
mcvol	143.850	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook

rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1485.00		NIST Webbook
tb	547.94	K	Joback Method
tc	763.06	K	Joback Method
tf	373.07	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.95	J/mol×K	547.94	Joback Method
cpg	360.43	J/mol×K	583.79	Joback Method
cpg	373.90	J/mol×K	619.65	Joback Method
cpg	386.47	J/mol×K	655.50	Joback Method
cpg	398.20	J/mol×K	691.35	Joback Method
cpg	409.19	J/mol×K	727.20	Joback Method
cpg	419.51	J/mol×K	763.06	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C539151&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