Oxymetazoline

Other names: Phenol, 3-[(4,5-dihydro-1H-imidazol-2-yl)methyl]-6-(1,1-dimethylethyl)-2,4-dimethyl-
Phenol, 6-tert-butyl-3-(2-imidazolin-2-ylmethyl)-2,4-dimethyl-
Hazol
Iliadin
Nafrine
Navisin
Nezeril
Oxylazine
Oxymethazoline
Oxymetozoline
Sinerol
Phenol, 6-t-butyl-3-(2-imidazolin-2-ylmethyl)-2,4-dimethyl-
6-t-Butyl-3-(2-imidazolin-2-ylmethyl)-2,4-dimethylphenol
3-[(4,5-Dihydro-1H-imidazol-2-yl)methyl]-6-(1,1-dimethylethyl)-2,4-dimethylphenol
6-tert-Butyl-3-(2-imidazolin-2-ylmethyl)-2,4-dimethylphenol
H-990
Navasin
Rhinofrenol
Rhinolitan
2-(4-tert-Butyl-2,6-dimethyl-3-hydroxybenzyl)-2-imidazoline

Inchi: InChI=1S/C16H24N2O/c1-10-8-13(16(3,4)5)15(19)11(2)12(10)9-14-17-6-7-18-14/h8,19H

InchiKey: WYWIFABBXFUGLM-UHFFFAOYSA-N

Formula: C16H24N2O

SMILES: Cc1cc(C(C)(C)C)c(O)c(C)c1CC1=NCCN1

Mol. weight [g/mol]: 260.37

CAS: 1491-59-4

Physical Properties

Property code	Value	Unit	Source
gf	284.66	kJ/mol	Joback Method
hf	-121.60	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	81.68	kJ/mol	Joback Method
ie	8.36	eV	NIST Webbook
log10ws	-3.67		Crippen Method
logp	2.851		Crippen Method
mcvol	223.210	ml/mol	McGowan Method

pc	2402.92	kPa	Joback Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
rinpol	2170.00		NIST Webbook
tb	810.83	K	Joback Method
tc	1059.46	K	Joback Method
tf	653.19	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.39	J/mol×K	810.83	Joback Method
cpg	714.98	J/mol×K	852.27	Joback Method
cpg	731.42	J/mol×K	893.71	Joback Method
cpg	746.83	J/mol×K	935.15	Joback Method
cpg	761.34	J/mol×K	976.58	Joback Method
cpg	775.06	J/mol×K	1018.02	Joback Method
cpg	788.12	J/mol×K	1059.46	Joback Method

Sources

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=C1491594&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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