Perillartine

Other names:	1-Cyclohexene-1-carboxaldehyde, 4-(1-methylethenyl)-, oxime, (E)-
	1-Cyclohexene-1-carboxaldehyde, 4-isopropenyl-, anti-oxime
	4-Isopropenyl-1-cyclohexene-1-carboxaldehyde, anti-oxime
	1-Perillaldehyde «alpha»-antioxime
	l-Perillaldehyde «alpha»-syn-oxime
	Perilla sugar
	(E)-4-(1-methylvinyl)cyclohexene-1-carbaldehyde oxime
Inchi:	InChI=1S/C10H15NO/c1-8(2)10-5-3-9(4-6-10)7-11-12/h3,7,10,12H,1,4-6H2,2H3
InchiKey:	XCOJIVIDDFTHGB-UHFFFAOYSA-N
Formula:	C10H15NO
SMILES:	C=C(C)C1CC=C(C=NO)CC1
Mol. weight [g/mol]:	165.23
CAS:	30950-27-7

Physical Properties

Property code	Value	Unit	Source
hf	-103.47	kJ/mol	Joback Method
hvap	58.64	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.749		Crippen Method
mcvol	143.850	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	617.31	K	Joback Method
tc	828.74	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30950277&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

Legend

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature