Benzofuran, 4,5,6,7-tetrahydro-3,6-dimethyl-

Other names:	(+)-menthofuran
	(R)-3,6-dimethyl-4,5,6,7-tetrahydrobenzofuran
	(R)-menthofuran
	3,6-Dimethyl-4,5,6,7-tetrahydro-1-benzofuran
	3,9-Epoxy-p-mentha-3,8-diene
	4,5,6,7-Tetrahydro-3,6-dimethylbenzofuran
	Menthofuran
	Menthofurane
	p-Mentha-3,8-diene, 3,9-epoxy-
Inchi:	InChI=1S/C10H14O/c1-7-3-4-9-8(2)6-11-10(9)5-7/h6-7H,3-5H2,1-2H3
InchiKey:	YGWKXXYGDYYFJU-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	Cc1coc2c1CCC(C)C2
Mol. weight [g/mol]:	150.22
CAS:	494-90-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.36		Crippen Method
logp	2.713		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
rinpol	1147.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1157.90		NIST Webbook

rinpol	1171.00	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1187.00	NIST Webbook
rinpol	1164.00	NIST Webbook
rinpol	1163.00	NIST Webbook
rinpol	1152.00	NIST Webbook
rinpol	1164.00	NIST Webbook
rinpol	1164.00	NIST Webbook
rinpol	1153.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1166.00	NIST Webbook
rinpol	1163.00	NIST Webbook
rinpol	1165.00	NIST Webbook
rinpol	1169.00	NIST Webbook
rinpol	1183.00	NIST Webbook
rinpol	1165.00	NIST Webbook
ripol	1487.00	NIST Webbook
ripol	1487.00	NIST Webbook
ripol	1478.00	NIST Webbook
ripol	1477.00	NIST Webbook
ripol	1483.00	NIST Webbook
ripol	1502.00	NIST Webbook
ripol	1497.00	NIST Webbook
ripol	1460.00	NIST Webbook
ripol	1487.00	NIST Webbook
ripol	1503.00	NIST Webbook
ripol	1458.00	NIST Webbook
ripol	1503.00	NIST Webbook
ripol	1458.00	NIST Webbook
ripol	1477.00	NIST Webbook
ripol	1487.00	NIST Webbook
ripol	1503.00	NIST Webbook
ripol	1490.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hvapt	56.50	kJ/mol	298.15	The vapor pressure and vaporization enthalpy of R-(+)-menthofuran, a hepatotoxin metabolically derived from the abortifacient terpene, (R)-(+)-pulegone by correlation gas chromatography

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The vapor pressure and vaporization enthalpy of R-(+)-menthofuran, a hepatotoxin metabolically derived from the abortifacient terpene, (R)-(+)-pulegone by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2016.03.020
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C494906&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices