Ethyl maltol

Other names:	2-Ethyl-3-hydroxy-4-pyrone
	2-Ethyl-3-hydroxy-4H-pyran-4-one
	2-Ethylpyromeconic acid
	3-Hydroxy-2-ethyl-1,4-pyrone
	3-Hydroxy-2-ethyl-4-pyrone
	3-Hydroxy-2-ethyl-4H-pyran-4-one
	3-Hydroxy-2-ethyl-«gamma»-pyrone
	3-Hydroxy-2-ethyl-Â«gammaÂ»-pyrone
	4H-Pyran-4-one, 2-ethyl-3-hydroxy-
	Veltol plus
Inchi:	InChI=1S/C7H8O3/c1-2-6-7(9)5(8)3-4-10-6/h3-4,9H,2H2,1H3
InchiKey:	YIKYNHJUKRTCJL-UHFFFAOYSA-N
Formula:	C7H8O3
SMILES:	CCc1occc(=O)c1O
Mol. weight [g/mol]:	140.14
CAS:	4940-11-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.89		Aqueous Solubility Prediction Method
logp	0.908		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
rinpol	1193.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1199.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2052.00		NIST Webbook
ripol	2052.00		NIST Webbook
ripol	2050.00		NIST Webbook
tf	364.17	K	Solubility of Ethyl Maltol in Aqueous Ethanol Mixtures

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	91.40	kJ/mol	298.15	When theory and experiment hold hands: The thermochemistry of gamma-pyrone derivatives

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4940118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
When theory and experiment hold hands: The thermochemistry of gamma-pyrone derivatives:	https://www.doi.org/10.1016/j.jct.2011.02.021
Solubility of Ethyl Maltol in Aqueous Ethanol Mixtures:	https://www.doi.org/10.1021/je800600q

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
tf:	Normal melting (fusion) point