2H-Pyran-2-one, 6-pentyl-

Other names:	6-Amyl-«alpha»-pyrone
	Pyran-2-one, 6-pentyl-
	6-N-Amyl «alpha»-pyrone
	6-Pentyl-2H-pyran-2-one
	«alpha»-Pyrone, 6-pentyl
	2-Pyrone, 6-pentyl
	6-Pentyl-«alpha»-pyrone
	«delta»-Deca-2,4-dienolactone
Inchi:	InChI=1S/C10H14O2/c1-2-3-4-6-9-7-5-8-10(11)12-9/h5,7-8H,2-4,6H2,1H3
InchiKey:	MAUFTTLGOUBZNA-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	CCCCCc1cccc(=O)o1
Mol. weight [g/mol]:	166.22
CAS:	27593-23-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.69		Crippen Method
logp	2.372		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1450.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1406.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2143.00		NIST Webbook
ripol	2143.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2163.00		NIST Webbook
ripol	2164.00		NIST Webbook
ripol	2166.00		NIST Webbook
ripol	2175.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27593233&Units=SI

Legend

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