Massoilactone

Other names:	2H-Pyran-2-one, 5,6-dihydro-6-pentyl-, (R)-
	(R)-(-)-Massoilactone
	Massoia lactone
	6-Pentyl-5,6-dihydro-2H-pyran-2-one, (6R)-
	5,6-Dihydro-6-pentyl-(2H)-pyran-2-one-, (R)
	Massoya lactone
	Cocolactone
	5,6-Dihydro-6-pentyl-(2H)-pyran-2-one, massoi lactone
	2H-Pyran-2-one, 5,6-dihydro-6-pentyl-, (6R)-
	5-Pentylpent-2-en-5-olide
	6-pentyl-5,6-dihydropyran-2-one
Inchi:	InChI=1S/C10H16O2/c1-2-3-4-6-9-7-5-8-10(11)12-9/h5,8-9H,2-4,6-7H2,1H3
InchiKey:	NEDIAPMWNCQWNW-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CCCCCC1CC=CC(=O)O1
Mol. weight [g/mol]:	168.23
CAS:	51154-96-2

Physical Properties

Property code	Value	Unit	Source
gf	-120.98	kJ/mol	Joback Method
hf	-407.33	kJ/mol	Joback Method
hfus	22.20	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.438		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	1433.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1446.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2241.00		NIST Webbook

ripol	2255.00		NIST Webbook
ripol	2247.00		NIST Webbook
ripol	2247.00		NIST Webbook
ripol	2241.00		NIST Webbook
tb	541.68	K	Joback Method
tc	755.53	K	Joback Method
tf	305.39	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.39	J/mol×K	541.68	Joback Method
cpg	369.45	J/mol×K	577.32	Joback Method
cpg	385.67	J/mol×K	612.96	Joback Method
cpg	401.05	J/mol×K	648.61	Joback Method
cpg	415.58	J/mol×K	684.25	Joback Method
cpg	429.28	J/mol×K	719.89	Joback Method
cpg	442.14	J/mol×K	755.53	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51154962&Units=SI

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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume