

D-lactone of 5-hydroxy-2-hexenoic acid

Inchi:	InChI=1S/C6H8O2/c1-5-3-2-4-6(7)8-5/h2,4-5H,3H2,1H3
InchiKey:	DYNKRGCMLGUEMN-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	CC1CC=CC(=O)O1
Mol. weight [g/mol]:	112.13
CAS:	108-54-3

Physical Properties

Property code	Value	Unit	Source
gf	-154.66	kJ/mol	Joback Method
hf	-324.77	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	38.43	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.878		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4288.66	kPa	Joback Method
tb	450.16	K	Joback Method
tc	678.51	K	Joback Method
tf	260.31	K	Joback Method
vc	0.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.07	J/molxK	450.16	Joback Method
cpg	189.67	J/molxK	488.22	Joback Method
cpg	201.74	J/molxK	526.28	Joback Method
cpg	213.26	J/molxK	564.33	Joback Method
cpg	224.23	J/molxK	602.39	Joback Method
cpg	234.62	J/molxK	640.45	Joback Method
cpg	244.41	J/molxK	678.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108543&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

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

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