

Dehydromevalonic lactone

Other names:	2H-Pyran-2-one, 5,6-dihydro-4-methyl-Mevalonic lactone, «DELTA»2-anhydro-2,3-Anhydromevalonic acid «delta»-lactone 2-Pentenoic acid, 5-hydroxy-3-methyl-, lactone 5,6-Dihydro-4-methyl-(2H)-pyran-2-one, dehydromevalonic acid lactone
Inchi:	InChI=1S/C6H8O2/c1-5-2-3-8-6(7)4-5/h4H,2-3H2,1H3
InchiKey:	RPEASMBBMVIKUTH-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	CC1=CC(=O)OCC1
Mol. weight [g/mol]:	112.13
CAS:	2381-87-5

Physical Properties

Property code	Value	Unit	Source
gf	-156.58	kJ/mol	Joback Method
hf	-315.90	kJ/mol	Joback Method
hfus	10.38	kJ/mol	Joback Method
hvap	39.40	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.880		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
rinpol	1169.30		NIST Webbook
rinpol	1169.30		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1114.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1978.00		NIST Webbook
ripol	1967.00		NIST Webbook
tb	459.81	K	Joback Method
tc	689.89	K	Joback Method
tf	277.07	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.28	J/mol×K	459.81	Joback Method
cpg	188.09	J/mol×K	498.16	Joback Method
cpg	199.41	J/mol×K	536.50	Joback Method
cpg	210.21	J/mol×K	574.85	Joback Method
cpg	220.50	J/mol×K	613.20	Joback Method
cpg	230.25	J/mol×K	651.55	Joback Method
cpg	239.44	J/mol×K	689.89	Joback Method

Sources

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=C2381875&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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