

4-Vinyl-4-hydroxypentalactone

Inchi:	InChI=1S/C8H12O2/c1-3-8(2)4-5-10-7(9)6-8/h3H,1,4-6H2,2H3
InchiKey:	ZOTMZCFLRCZZED-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	C=CC1(C)CCOC(=O)C1
Mol. weight [g/mol]:	140.18

Physical Properties

Property code	Value	Unit	Source
gf	-85.43	kJ/mol	Joback Method
hf	-283.16	kJ/mol	Joback Method
hfus	8.22	kJ/mol	Joback Method
hvap	40.77	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.516		Crippen Method
mvol	115.860	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
ripol	1658.00		NIST Webbook
ripol	1658.00		NIST Webbook
tb	493.68	K	Joback Method
tc	727.53	K	Joback Method
tf	304.23	K	Joback Method
vc	0.423	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.83	J/mol×K	493.68	Joback Method
cpg	275.53	J/mol×K	532.65	Joback Method
cpg	290.23	J/mol×K	571.63	Joback Method
cpg	304.02	J/mol×K	610.60	Joback Method
cpg	317.01	J/mol×K	649.58	Joback Method
cpg	329.30	J/mol×K	688.55	Joback Method
cpg	340.99	J/mol×K	727.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410478&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
ri pol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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