

(Z)-Whisky lactone

Inchi:	InChI=1S/C9H16O2/c1-3-4-5-8-7(2)6-9(10)11-8/h7-8H,3-6H2,1-2H3
InchiKey:	WNVCMFHPRIBNCW-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	CCCCC1OC(=O)CC1C
Mol. weight [g/mol]:	156.22

Physical Properties

Property code	Value	Unit	Source
gf	-154.97	kJ/mol	Joback Method
hf	-458.65	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	44.33	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.128		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
ripol	1957.00		NIST Webbook
ripol	1957.00		NIST Webbook
tb	510.70	K	Joback Method
tc	718.10	K	Joback Method
tf	292.64	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.83	J/molxK	510.70	Joback Method
cpg	340.60	J/molxK	545.27	Joback Method
cpg	356.64	J/molxK	579.83	Joback Method
cpg	371.95	J/molxK	614.40	Joback Method
cpg	386.53	J/molxK	648.97	Joback Method
cpg	400.37	J/molxK	683.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R618236&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

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