

C9H14O

Inchi:	InChI=1S/C9H14O/c1-7-3-4-9(6-10)5-8(7)2/h6,9H,3-5H2,1-2H3
InchiKey:	NOJNKSAQZMVMFF-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC1=C(C)CC(C=O)CC1
Mol. weight [g/mol]:	138.21
CAS:	93861-86-0

Physical Properties

Property code	Value	Unit	Source
gf	-39.47	kJ/mol	Joback Method
hf	-225.51	kJ/mol	Joback Method
hfus	13.63	kJ/mol	Joback Method
hvap	44.39	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
tb	482.65	K	Joback Method
tc	692.10	K	Joback Method
tf	266.37	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.51	J/molxK	482.65	Joback Method
cpg	283.55	J/molxK	517.56	Joback Method
cpg	297.84	J/molxK	552.47	Joback Method
cpg	311.42	J/molxK	587.38	Joback Method
cpg	324.28	J/molxK	622.29	Joback Method
cpg	336.45	J/molxK	657.19	Joback Method
cpg	347.94	J/molxK	692.10	Joback Method
dvisc	0.0026032	Paxs	266.37	Joback Method
dvisc	0.0014704	Paxs	302.42	Joback Method

dvisc	0.0009380	Paxs	338.46	Joback Method
dvisc	0.0006525	Paxs	374.51	Joback Method
dvisc	0.0004837	Paxs	410.56	Joback Method
dvisc	0.0003764	Paxs	446.60	Joback Method
dvisc	0.0003040	Paxs	482.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93861860&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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