

C9H10O

Inchi:	InChI=1S/C9H10O/c1-8(7-10)9-5-3-2-4-6-9/h2-8H,1H3
InchiKey:	IQVAERDLDAZARL-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	CC(C=O)c1ccccc1
Mol. weight [g/mol]:	134.18
CAS:	34713-70-7

Physical Properties

Property code	Value	Unit	Source
gf	35.35	kJ/mol	Joback Method
hf	-83.42	kJ/mol	Joback Method
hfus	11.87	kJ/mol	Joback Method
hvap	44.24	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.989		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
tb	480.22	K	Joback Method
tc	697.92	K	Joback Method
tf	244.61	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.06	J/molxK	480.22	Joback Method
cpg	248.02	J/molxK	516.50	Joback Method
cpg	260.17	J/molxK	552.79	Joback Method
cpg	271.54	J/molxK	589.07	Joback Method
cpg	282.17	J/molxK	625.36	Joback Method
cpg	292.08	J/molxK	661.64	Joback Method
cpg	301.32	J/molxK	697.92	Joback Method
dvisc	0.0048271	Paxs	244.61	Joback Method
dvisc	0.0021603	Paxs	283.88	Joback Method

dvisc	0.0011754	Paxs	323.15	Joback Method
dvisc	0.0007297	Paxs	362.41	Joback Method
dvisc	0.0004973	Paxs	401.68	Joback Method
dvisc	0.0003628	Paxs	440.95	Joback Method
dvisc	0.0002787	Paxs	480.22	Joback Method

Sources

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=C34713707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	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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