3',4'-(Methylenedioxy)acetophenone

Other names:	1-(1,3-benzodioxol-5-yl)ethan-1-one
	3,4-Methylen-dioxy-acetophenon
	3,4-Methylenedioxyacetophenone
	3,4-Methylenedioxycetophenone
	5-oxoethyl-1,3-benzodioxole
	Acetopiperone
	Ethanone, 1-(1,3-benzodioxol-5-yl)-
Inchi:	InChI=1S/C9H8O3/c1-6(10)7-2-3-8-9(4-7)12-5-11-8/h2-4H,5H2,1H3
InchiKey:	BMHMKWXYXFBWMI-UHFFFAOYSA-N
Formula:	C9H8O3
SMILES:	CC(=O)c1ccc2c(c1)OCO2
Mol. weight [g/mol]:	164.16
CAS:	3162-29-6

Physical Properties

Property code	Value	Unit	Source
gf	-114.65	kJ/mol	Joback Method
hf	-298.94	kJ/mol	Joback Method
hfus	26.23	kJ/mol	Experimental and Computational Thermochemistry of 1,3-Benzodioxole Derivatives
hsub	104.40 ± 2.20	kJ/mol	NIST Webbook
hvap	55.22	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.618		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	561.14	K	Joback Method
tc	795.13	K	Joback Method
tf	367.90	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.26	J/mol×K	795.13	Joback Method
cpg	270.65	J/mol×K	561.14	Joback Method
cpg	282.02	J/mol×K	600.14	Joback Method
cpg	292.53	J/mol×K	639.14	Joback Method
cpg	302.25	J/mol×K	678.14	Joback Method
cpg	311.24	J/mol×K	717.14	Joback Method
cpg	319.56	J/mol×K	756.14	Joback Method
dvisc	0.0005344	Pa×s	561.14	Joback Method
dvisc	0.0022182	Pa×s	367.90	Joback Method
dvisc	0.0015904	Pa×s	400.11	Joback Method
dvisc	0.0011982	Pa×s	432.31	Joback Method
dvisc	0.0009389	Pa×s	464.52	Joback Method
dvisc	0.0007594	Pa×s	496.73	Joback Method
dvisc	0.0006303	Pa×s	528.93	Joback Method
hfust	26.23	kJ/mol	358.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	426.50 ± 1.50	K	2.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3162296&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Experimental and Computational Thermochemistry of 1,3-Benzodioxole Derivatives: https://www.doi.org/10.1021/je700035m

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume