3,4-Methylenedioxyphenyl acetone

Other names:	(3,4-(Methylenedioxy)phenyl)-2-propanone
	2-Propanone, 1-(1,3-benzodioxol-5-yl)-
	Methyl piperonyl ketone
	1-(Acetonyl)-3,4-methylenedioxybenzene
	2-Propanone, (3,4-(methylenedioxy)phenyl)-
	2-Propanone, 1-(3,4-(methylenedioxy)phenyl)-
	3,4-Methylenedioxybenzyl methyl ketone
	5-Acetonyl-1,3-benzodioxole
	2-Propanone, 1-[1,3-benzodioxo-5-yl]-
	(1,3-Benzodioxolan-5-yl)acetone
	NSC 16688
	1-(1,3-benzodioxol-5-yl)acetone
Inchi:	InChI=1S/C10H10O3/c1-7(11)4-8-2-3-9-10(5-8)13-6-12-9/h2-3,5H,4,6H2,1H3
InchiKey:	XIYKRJLTYKUWAM-UHFFFAOYSA-N
Formula:	C10H10O3
SMILES:	CC(=O)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	178.18
CAS:	4676-39-5

Physical Properties

Property code	Value	Unit	Source
gf	-106.23	kJ/mol	Joback Method
hf	-319.58	kJ/mol	Joback Method
hfus	29.54	kJ/mol	Joback Method
hvap	57.44	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.547		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
tb	557.00 ± 4.00	K	NIST Webbook
tb	557.00 ± 3.00	K	NIST Webbook
tc	813.44	K	Joback Method
tf	379.17	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.82	J/mol×K	584.02	Joback Method
cpg	328.09	J/mol×K	622.26	Joback Method
cpg	339.48	J/mol×K	660.49	Joback Method
cpg	350.06	J/mol×K	698.73	Joback Method
cpg	359.87	J/mol×K	736.97	Joback Method
cpg	368.99	J/mol×K	775.21	Joback Method
cpg	377.47	J/mol×K	813.44	Joback Method
dvisc	0.0022370	Pa×s	379.17	Joback Method
dvisc	0.0015736	Pa×s	413.31	Joback Method
dvisc	0.0011680	Pa×s	447.45	Joback Method
dvisc	0.0009043	Pa×s	481.60	Joback Method
dvisc	0.0007243	Pa×s	515.74	Joback Method
dvisc	0.0005964	Pa×s	549.88	Joback Method
dvisc	0.0005023	Pa×s	584.02	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4676395&Units=SI

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