3,4-Methylenedioxypropiophenone

Other names:	1-Propanone, 1-(1,3-benzodioxol-5-yl)-
	1-(1,3-Benzodioxol-5-yl)-1-propanone
	3',4'-Methylenedioxypropiophenone
	NSC 29484
	1-(1,3-benzodioxol-5-yl)propan-1-one
Inchi:	InChI=1S/C10H10O3/c1-2-8(11)7-3-4-9-10(5-7)13-6-12-9/h3-5H,2,6H2,1H3
InchiKey:	RVBJGSPBFIUTTR-UHFFFAOYSA-N
Formula:	C10H10O3
SMILES:	CCC(=O)c1ccc2c(c1)OCO2
Mol. weight [g/mol]:	178.18
CAS:	28281-49-4

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	-2.76		Crippen Method
logp	2.008		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
tb	584.02	K	Joback Method
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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	439.50 ± 1.50	K	2.70	NIST Webbook

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=C28281494&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume