1,2-propanedione,1-(3,4-methylenedioxy)phenyl

Other names: R,S-3',4'-methylenedioxy-«alpha»-pyrrolidinopropiophenone-M (desamino-oxo-)
Inchi: InChI=1S/C10H8O4/c1-6(11)10(12)7-2-3-8-9(4-7)14-5-13-8/h2-4H,5H2,1H3
InchiKey: FGXKZQWZZVCYBF-UHFFFAOYSA-N
Formula: C10H8O4
SMILES: CC(=O)C(=O)c1ccc2c(c1)OCO2
Mol. weight [g/mol]: 192.17

Physical Properties

Property code	Value	Unit	Source
gf	-235.15	kJ/mol	Joback Method
hf	-432.16	kJ/mol	Joback Method
hfus	31.14	kJ/mol	Joback Method
hvap	64.19	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.187		Crippen Method
mcvol	132.020	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
rinpol	1525.00		NIST Webbook
tb	637.89	K	Joback Method
tc	874.30	K	Joback Method
tf	429.10	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.61	J/mol×K	637.89	Joback Method
cpg	373.72	J/mol×K	834.90	Joback Method
cpg	365.93	J/mol×K	795.49	Joback Method
cpg	357.48	J/mol×K	756.09	Joback Method
cpg	348.32	J/mol×K	716.69	Joback Method
cpg	338.39	J/mol×K	677.29	Joback Method
cpg	380.94	J/mol×K	874.30	Joback Method
dvisc	0.0005425	Pa×s	637.89	Joback Method

dvisc	0.0006419	Pa×s	603.09	Joback Method
dvisc	0.0007755	Pa×s	568.29	Joback Method
dvisc	0.0009601	Pa×s	533.50	Joback Method
dvisc	0.0012247	Pa×s	498.70	Joback Method
dvisc	0.0016203	Pa×s	463.90	Joback Method
dvisc	0.0022432	Pa×s	429.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378930&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume