Methyl 6-hydroxy-2-methyl-3,4-methylenedioxy-benzoate acetylated

Inchi: InChI=1S/C12H12O6/c1-6-10(12(14)15-3)8(18-7(2)13)4-9-11(6)17-5-16-9/h4H,5H2,1-3H
InchiKey: ACGCOIAOACSKAM-UHFFFAOYSA-N
Formula: C12H12O6
SMILES: COC(=O)c1c(OC(C)=O)cc2c(c1C)OCO2
Mol. weight [g/mol]: 252.22

Physical Properties

Property code	Value	Unit	Source
gf	-447.57	kJ/mol	Joback Method
hf	-760.82	kJ/mol	Joback Method
hfus	37.92	kJ/mol	Joback Method
hvap	74.78	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	1.436		Crippen Method
mcvol	171.940	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	1761.00		NIST Webbook
tb	738.45	K	Joback Method
tc	961.73	K	Joback Method
tf	521.14	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.61	J/mol×K	738.45	Joback Method
cpg	482.10	J/mol×K	775.66	Joback Method
cpg	492.78	J/mol×K	812.88	Joback Method
cpg	502.69	J/mol×K	850.09	Joback Method
cpg	511.82	J/mol×K	887.31	Joback Method
cpg	520.19	J/mol×K	924.52	Joback Method
cpg	527.82	J/mol×K	961.73	Joback Method
dvisc	0.0009657	Pa×s	521.14	Joback Method
dvisc	0.0007349	Pa×s	557.36	Joback Method

dvisc	0.0005781	Pa×s	593.58	Joback Method
dvisc	0.0004676	Pa×s	629.80	Joback Method
dvisc	0.0003870	Pa×s	666.01	Joback Method
dvisc	0.0003266	Pa×s	702.23	Joback Method
dvisc	0.0002803	Pa×s	738.45	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=R273917&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume