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

Inchi: InChI=1S/C10H10O5/c1-5-8(10(12)13-2)6(11)3-7-9(5)15-4-14-7/h3,11H,4H2,1-2H3

InchiKey: VPYDVSWMSWPSKV-UHFFFAOYSA-N

Formula: C10H10O5

SMILES: COC(=O)c1c(O)cc2c(c1C)OCO2

Mol. weight [g/mol]: 210.18

Physical Properties

Property code	Value	Unit	Source
gf	-375.48	kJ/mol	Joback Method
hf	-640.58	kJ/mol	Joback Method
hfus	36.12	kJ/mol	Joback Method
hvap	73.53	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.216		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	1626.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1618.00		NIST Webbook
tb	692.04	K	Joback Method
tc	927.74	K	Joback Method
tf	525.64	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.42	J/mol×K	692.04	Joback Method
cpg	391.69	J/mol×K	731.32	Joback Method
cpg	401.33	J/mol×K	770.61	Joback Method
cpg	410.43	J/mol×K	809.89	Joback Method
cpg	419.08	J/mol×K	849.17	Joback Method
cpg	427.36	J/mol×K	888.45	Joback Method
cpg	435.37	J/mol×K	927.74	Joback Method

dvisc	0.0002744	Pa×s	525.64	Joback Method
dvisc	0.0001839	Pa×s	553.37	Joback Method
dvisc	0.0001280	Pa×s	581.11	Joback Method
dvisc	0.0000921	Pa×s	608.84	Joback Method
dvisc	0.0000682	Pa×s	636.57	Joback Method
dvisc	0.0000518	Pa×s	664.31	Joback Method
dvisc	0.0000402	Pa×s	692.04	Joback Method

Sources

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=R273902&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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