3-Hydroxy-4-methoxybenzyl alcohol, di(acetate)

Inchi: InChI=1S/C12H14O5/c1-8(13)16-7-10-4-5-11(15-3)12(6-10)17-9(2)14/h4-6H,7H2,1-3H3
InchiKey: SRSODAZXLUDDDY-UHFFFAOYSA-N
Formula: C12H14O5
SMILES: COc1ccc(COC(C)=O)cc1OC(C)=O
Mol. weight [g/mol]: 238.24

Physical Properties

Property code	Value	Unit	Source
gf	-429.53	kJ/mol	Joback Method
hf	-699.24	kJ/mol	Joback Method
hfus	26.86	kJ/mol	Joback Method
hvap	66.63	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.684		Crippen Method
mcvol	176.930	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1746.00		NIST Webbook
tb	685.60	K	Joback Method
tc	896.10	K	Joback Method
tf	443.01	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.63	J/mol×K	685.60	Joback Method
cpg	517.48	J/mol×K	861.01	Joback Method
cpg	507.76	J/mol×K	825.93	Joback Method
cpg	497.19	J/mol×K	790.85	Joback Method
cpg	485.80	J/mol×K	755.77	Joback Method
cpg	473.61	J/mol×K	720.68	Joback Method
cpg	526.34	J/mol×K	896.10	Joback Method
dvisc	0.0001162	Pa×s	685.60	Joback Method
dvisc	0.0001425	Pa×s	645.17	Joback Method

dvisc	0.0001795	Pa×s	604.74	Joback Method
dvisc	0.0002338	Pa×s	564.31	Joback Method
dvisc	0.0003171	Pa×s	523.87	Joback Method
dvisc	0.0004528	Pa×s	483.44	Joback Method
dvisc	0.0006897	Pa×s	443.01	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=U374289&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