3-(Acetyloxy)benzoic acetic anhydride

Inchi: InChI=1S/C11H10O5/c1-7(12)15-10-5-3-4-9(6-10)11(14)16-8(2)13/h3-6H,1-2H3
InchiKey: NBJUJOIKIGAIRE-UHFFFAOYSA-N
Formula: C11H10O5
SMILES: CC(=O)OC(=O)c1cccc(OC(C)=O)c1
Mol. weight [g/mol]: 222.19

Physical Properties

Property code	Value	Unit	Source
gf	-452.24	kJ/mol	Joback Method
hf	-647.49	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	68.08	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.315		Crippen Method
mcvol	158.540	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
tb	689.19	K	Joback Method
tc	910.86	K	Joback Method
tf	446.92	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.64	J/mol×K	689.19	Joback Method
cpg	410.96	J/mol×K	726.14	Joback Method
cpg	421.47	J/mol×K	763.08	Joback Method
cpg	431.17	J/mol×K	800.03	Joback Method
cpg	440.05	J/mol×K	836.97	Joback Method
cpg	448.10	J/mol×K	873.92	Joback Method
cpg	455.33	J/mol×K	910.86	Joback Method
dvisc	0.0010372	Pa×s	446.92	Joback Method

dvisc	0.0006757	Pa×s	487.30	Joback Method
dvisc	0.0004701	Pa×s	527.68	Joback Method
dvisc	0.0003443	Pa×s	568.06	Joback Method
dvisc	0.0002628	Pa×s	608.43	Joback Method
dvisc	0.0002075	Pa×s	648.81	Joback Method
dvisc	0.0001684	Pa×s	689.19	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=U375039&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