2-(Acetyloxy)-3-methoxybenzoic acid

Inchi: InChI=1S/C10H10O5/c1-6(11)15-9-7(10(12)13)4-3-5-8(9)14-2/h3-5H,1-2H3,(H,12,13)
InchiKey: GOBRPXJFIGHDQG-UHFFFAOYSA-N
Formula: C10H10O5
SMILES: COc1cccc(C(=O)O)c1OC(C)=O
Mol. weight [g/mol]: 210.18

Physical Properties

Property code	Value	Unit	Source
gf	-478.19	kJ/mol	Joback Method
hf	-677.97	kJ/mol	Joback Method
hfus	24.58	kJ/mol	Joback Method
hvap	76.44	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.319		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
rinpol	1781.00		NIST Webbook
tb	709.60	K	Joback Method
tc	914.96	K	Joback Method
tf	459.06	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.50	J/mol×K	709.60	Joback Method
cpg	393.06	J/mol×K	743.83	Joback Method
cpg	402.00	J/mol×K	778.05	Joback Method
cpg	410.31	J/mol×K	812.28	Joback Method
cpg	417.99	J/mol×K	846.50	Joback Method
cpg	425.01	J/mol×K	880.73	Joback Method
cpg	431.39	J/mol×K	914.96	Joback Method
dvisc	0.0007005	Pa×s	459.06	Joback Method
dvisc	0.0003617	Pa×s	500.82	Joback Method

dvisc	0.0002068	Pa×s	542.57	Joback Method
dvisc	0.0001280	Pa×s	584.33	Joback Method
dvisc	0.0000845	Pa×s	626.09	Joback Method
dvisc	0.0000588	Pa×s	667.84	Joback Method
dvisc	0.0000426	Pa×s	709.60	Joback Method

Sources

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=U352874&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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