Acetoxyacetic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C11H12O5/c1-8(12)15-7-11(13)16-10-5-3-9(14-2)4-6-10/h3-6H,7H2,1-2H3
InchiKey: RJDNAIXYTFIJPO-UHFFFAOYSA-N
Formula: C11H12O5
SMILES: COc1ccc(OC(=O)COC(C)=O)cc1
Mol. weight [g/mol]: 224.21

Physical Properties

Property code	Value	Unit	Source
gf	-428.32	kJ/mol	Joback Method
hf	-667.13	kJ/mol	Joback Method
hfus	24.66	kJ/mol	Joback Method
hvap	63.74	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.164		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
tb	657.74	K	Joback Method
tc	870.60	K	Joback Method
tf	419.22	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.26	J/mol×K	657.74	Joback Method
cpg	423.76	J/mol×K	693.22	Joback Method
cpg	435.51	J/mol×K	728.69	Joback Method
cpg	446.49	J/mol×K	764.17	Joback Method
cpg	456.69	J/mol×K	799.65	Joback Method
cpg	466.09	J/mol×K	835.12	Joback Method
cpg	474.67	J/mol×K	870.60	Joback Method
dvisc	0.0008661	Pa×s	419.22	Joback Method

dvisc	0.0005512	Pa×s	458.97	Joback Method
dvisc	0.0003770	Pa×s	498.73	Joback Method
dvisc	0.0002727	Pa×s	538.48	Joback Method
dvisc	0.0002063	Pa×s	578.23	Joback Method
dvisc	0.0001617	Pa×s	617.99	Joback Method
dvisc	0.0001306	Pa×s	657.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307542&Units=SI
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

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