

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:	<chem>COc1ccc(OC(=O)COC(C)=O)cc1</chem>
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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0005512	Paxs	458.97	Joback Method
dvisc	0.0003770	Paxs	498.73	Joback Method
dvisc	0.0002727	Paxs	538.48	Joback Method
dvisc	0.0002063	Paxs	578.23	Joback Method
dvisc	0.0001617	Paxs	617.99	Joback Method
dvisc	0.0001306	Paxs	657.74	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=U307542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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