Acetoxyacetic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C17H16O5/c1-13(18)20-12-17(19)22-16-9-7-15(8-10-16)21-11-14-5-3-2-4-6-14
InchiKey: JUNAIOZDTRIYAP-UHFFFAOYSA-N
Formula: C17H16O5
SMILES: CC(=O)OCC(=O)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 300.31

Physical Properties

Property code	Value	Unit	Source
gf	-265.39	kJ/mol	Joback Method
hf	-554.44	kJ/mol	Joback Method
hfus	34.24	kJ/mol	Joback Method
hvap	79.37	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.734		Crippen Method
mcvol	223.620	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	2308.00		NIST Webbook
rinpol	2308.00		NIST Webbook
tb	821.70	K	Joback Method
tc	1051.24	K	Joback Method
tf	513.26	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.10	J/mol×K	821.70	Joback Method
cpg	652.30	J/mol×K	859.96	Joback Method
cpg	664.23	J/mol×K	898.21	Joback Method
cpg	674.89	J/mol×K	936.47	Joback Method
cpg	684.29	J/mol×K	974.73	Joback Method
cpg	692.45	J/mol×K	1012.98	Joback Method
cpg	699.38	J/mol×K	1051.24	Joback Method
dvisc	0.0004870	Pa×s	513.26	Joback Method

dvisc	0.0002971	Pa×s	564.67	Joback Method
dvisc	0.0001969	Pa×s	616.07	Joback Method
dvisc	0.0001390	Pa×s	667.48	Joback Method
dvisc	0.0001031	Pa×s	718.89	Joback Method
dvisc	0.0000796	Pa×s	770.29	Joback Method
dvisc	0.0000635	Pa×s	821.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307547&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