Acetoxyacetic acid, phenylmethyl ester

Inchi: InChI=1S/C11H12O4/c1-9(12)14-8-11(13)15-7-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3
InchiKey: ODZBRLHIJUSHGV-UHFFFAOYSA-N
Formula: C11H12O4
SMILES: CC(=O)OCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 208.21

Physical Properties

Property code	Value	Unit	Source
gf	-313.69	kJ/mol	Joback Method
hf	-523.44	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	60.67	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.293		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
rinpol	1486.00		NIST Webbook
tb	630.34	K	Joback Method
tc	844.72	K	Joback Method
tf	384.47	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.86	J/mol×K	630.34	Joback Method
cpg	400.74	J/mol×K	666.07	Joback Method
cpg	412.83	J/mol×K	701.80	Joback Method
cpg	424.13	J/mol×K	737.53	Joback Method
cpg	434.64	J/mol×K	773.26	Joback Method
cpg	444.37	J/mol×K	808.99	Joback Method
cpg	453.32	J/mol×K	844.72	Joback Method
dvisc	0.0014354	Pa×s	384.47	Joback Method
dvisc	0.0008448	Pa×s	425.45	Joback Method

dvisc	0.0005457	Pa×s	466.43	Joback Method
dvisc	0.0003783	Pa×s	507.41	Joback Method
dvisc	0.0002770	Pa×s	548.38	Joback Method
dvisc	0.0002118	Pa×s	589.36	Joback Method
dvisc	0.0001677	Pa×s	630.34	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308342&Units=SI

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