

Acetoxyacetic acid, 4-biphenyl ester

Inchi:	InChI=1S/C16H14O4/c1-12(17)19-11-16(18)20-15-9-7-14(8-10-15)13-5-3-2-4-6-13/h2-10
InchiKey:	ILJICPLAOFRHH-UHFFFAOYSA-N
Formula:	C16H14O4
SMILES:	CC(=O)OCC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	270.28

Physical Properties

Property code	Value	Unit	Source
gf	-168.81	kJ/mol	Joback Method
hf	-401.58	kJ/mol	Joback Method
hfus	30.46	kJ/mol	Joback Method
hvap	74.74	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	2.822		Crippen Method
mvol	203.660	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	2236.00		NIST Webbook
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tb	776.40	K	Joback Method
tc	1012.27	K	Joback Method
tf	479.76	K	Joback Method
vc	0.763	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.48	J/molxK	776.40	Joback Method
cpg	614.29	J/molxK	972.96	Joback Method
cpg	605.44	J/molxK	933.65	Joback Method
cpg	595.46	J/molxK	894.34	Joback Method
cpg	584.33	J/molxK	855.02	Joback Method
cpg	572.01	J/molxK	815.71	Joback Method
cpg	622.03	J/molxK	1012.27	Joback Method
dvisc	0.0000946	Paxs	776.40	Joback Method

dvisc	0.0001185	Paxs	726.96	Joback Method
dvisc	0.0001534	Paxs	677.52	Joback Method
dvisc	0.0002067	Paxs	628.08	Joback Method
dvisc	0.0002932	Paxs	578.64	Joback Method
dvisc	0.0004440	Paxs	529.20	Joback Method
dvisc	0.0007322	Paxs	479.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355703&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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