Methyl benzilate

Other names:	Benzeneacetic acid, «alpha»-hydroxy-«alpha»-phenyl-, methyl ester
	Benzilic acid, methyl ester
	Methyl diphenylglycolate
	Methyl «alpha»-hydroxydiphenylacetate
	Methyl «alpha»-phenylmandelate
	Methyl 2-hydroxy-2,2-diphenylacetate
	Methyl hydroxydiphenylacetate
	Hydroxy-diphenyl-acetic acid methyl ester
	«alpha»-Hydroxydiphenylacetic acid, methyl ester
	NSC 57672
Inchi:	InChI=1S/C15H14O3/c1-18-14(16)15(17,12-8-4-2-5-9-12)13-10-6-3-7-11-13/h2-11,17H,1
InchiKey:	LJFIHTFNTGQZJL-UHFFFAOYSA-N
Formula:	C15H14O3
SMILES:	COC(=O)C(O)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	242.27
CAS:	76-89-1

Physical Properties

Property code	Value	Unit	Source
gf	-67.66	kJ/mol	Joback Method
hf	-285.65	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	78.08	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.095		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	1805.00		NIST Webbook
rinpol	1792.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook
ripol	2833.00		NIST Webbook
ripol	2852.00		NIST Webbook
tb	761.20	K	Joback Method
tc	991.88	K	Joback Method
tf	347.50 ± 0.50	K	NIST Webbook

vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.81	J/mol×K	761.20	Joback Method
cpg	534.28	J/mol×K	799.65	Joback Method
cpg	545.67	J/mol×K	838.09	Joback Method
cpg	556.08	J/mol×K	876.54	Joback Method
cpg	565.59	J/mol×K	914.99	Joback Method
cpg	574.27	J/mol×K	953.43	Joback Method
cpg	582.21	J/mol×K	991.88	Joback Method
dvisc	0.0010065	Pa×s	447.05	Joback Method
dvisc	0.0003832	Pa×s	499.41	Joback Method
dvisc	0.0001752	Pa×s	551.77	Joback Method
dvisc	0.0000918	Pa×s	604.12	Joback Method
dvisc	0.0000533	Pa×s	656.48	Joback Method
dvisc	0.0000335	Pa×s	708.84	Joback Method
dvisc	0.0000225	Pa×s	761.20	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	460.20	K	1.70	NIST Webbook
tbrp	460.00	K	1.70	NIST Webbook

Sources

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=C76891&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume