Benzeneacetic acid, «alpha»-oxo-, methyl ester

Other names:	Methyl benzoylformate
	Methyl phenylglyoxylate
	Methyl phenylglyoxalate
	Benzoylformic acid methyl ester
	Glyoxylic acid, phenyl-, methyl ester
	Methyl oxophenylacetate
	Phenylglyoxylic acid, methyl ester
	Vicure 55
	«alpha»-Oxobenzeneacetic acid methyl ester
	NSC 171206
	Methyl 2-oxo-2-phenylacetate
Inchi:	InChI=1S/C9H8O3/c1-12-9(11)8(10)7-5-3-2-4-6-7/h2-6H,1H3
InchiKey:	YLHXLHGIAMFFBU-UHFFFAOYSA-N
Formula:	C9H8O3
SMILES:	COC(=O)C(=O)c1ccccc1
Mol. weight [g/mol]:	164.16
CAS:	15206-55-0

Physical Properties

Property code	Value	Unit	Source
gf	-225.53	kJ/mol	Joback Method
hf	-349.94	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	53.81	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.042		Crippen Method
mcvol	122.920	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
rinpol	1335.10		NIST Webbook
tb	520.20	K	NIST Webbook
tc	787.10	K	Joback Method
tf	339.70	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.90	J/mol×K	562.16	Joback Method
cpg	282.33	J/mol×K	599.65	Joback Method
cpg	293.03	J/mol×K	637.14	Joback Method
cpg	303.00	J/mol×K	674.63	Joback Method
cpg	312.27	J/mol×K	712.12	Joback Method
cpg	320.86	J/mol×K	749.61	Joback Method
cpg	328.77	J/mol×K	787.10	Joback Method
dvisc	0.0020532	Pa×s	339.70	Joback Method
dvisc	0.0012169	Pa×s	376.78	Joback Method
dvisc	0.0007921	Pa×s	413.85	Joback Method
dvisc	0.0005533	Pa×s	450.93	Joback Method
dvisc	0.0004082	Pa×s	488.01	Joback Method
dvisc	0.0003143	Pa×s	525.08	Joback Method
dvisc	0.0002505	Pa×s	562.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.20	K	1.90	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15206550&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume