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

Other names:	Glyoxylic acid, phenyl-, ethyl ester
	Ethyl benzoylformate
	Ethyl oxophenylacetate
	Ethyl phenylglyoxylate
	Ethyl 2-oxo-2-phenylacetate
	Phenylglyoxylic acid ethyl ester
Inchi:	InChI=1S/C10H10O3/c1-2-13-10(12)9(11)8-6-4-3-5-7-8/h3-7H,2H2,1H3
InchiKey:	QKLCQKPAECHXCQ-UHFFFAOYSA-N
Formula:	C10H10O3
SMILES:	CCOC(=O)C(=O)c1ccccc1
Mol. weight [g/mol]:	178.18
CAS:	1603-79-8

Physical Properties

Property code	Value	Unit	Source
gf	-217.11	kJ/mol	Joback Method
hf	-370.58	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	56.03	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.432		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	585.04	K	Joback Method
tc	805.88	K	Joback Method
tf	350.97	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.40	J/mol×K	585.04	Joback Method
cpg	370.44	J/mol×K	769.07	Joback Method
cpg	361.13	J/mol×K	732.27	Joback Method

cpg	351.09	J/mol×K	695.46	Joback Method
cpg	340.30	J/mol×K	658.65	Joback Method
cpg	328.74	J/mol×K	621.85	Joback Method
cpg	379.03	J/mol×K	805.88	Joback Method
dvisc	0.0002309	Pa×s	585.04	Joback Method
dvisc	0.0002912	Pa×s	546.03	Joback Method
dvisc	0.0003805	Pa×s	507.02	Joback Method
dvisc	0.0005201	Pa×s	468.00	Joback Method
dvisc	0.0007523	Pa×s	428.99	Joback Method
dvisc	0.0011717	Pa×s	389.98	Joback Method
dvisc	0.0020137	Pa×s	350.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.70	K	2.40	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=C1603798&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume