Butanoic acid, 3-oxo-, phenylmethyl ester

Other names:	Acetoacetic acid, benzyl ester
	Benzyl acetoacetate
	Benzyl acetylacetate
	Benzyl 3-oxobutanoate
	NSC 4391
	Phenylmethyl 3-oxobutanoate
Inchi:	InChI=1S/C11H12O3/c1-9(12)7-11(13)14-8-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3
InchiKey:	WOFAGNLBCJWEOE-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	CC(=O)CC(=O)OCc1ccccc1
Mol. weight [g/mol]:	192.21
CAS:	5396-89-4

Physical Properties

Property code	Value	Unit	Source
gf	-208.69	kJ/mol	Joback Method
hf	-391.22	kJ/mol	Joback Method
hfus	22.67	kJ/mol	Joback Method
hvap	58.26	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.709		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	607.92	K	Joback Method
tc	824.86	K	Joback Method
tf	362.24	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.58	J/mol×K	607.92	Joback Method
cpg	421.12	J/mol×K	788.70	Joback Method
cpg	411.19	J/mol×K	752.55	Joback Method

cpg	400.49	J/mol×K	716.39	Joback Method
cpg	389.01	J/mol×K	680.23	Joback Method
cpg	376.71	J/mol×K	644.08	Joback Method
cpg	430.30	J/mol×K	824.86	Joback Method
dvisc	0.0002109	Pa×s	607.92	Joback Method
dvisc	0.0002673	Pa×s	566.97	Joback Method
dvisc	0.0003514	Pa×s	526.03	Joback Method
dvisc	0.0004839	Pa×s	485.08	Joback Method
dvisc	0.0007070	Pa×s	444.13	Joback Method
dvisc	0.0011154	Pa×s	403.19	Joback Method
dvisc	0.0019508	Pa×s	362.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	430.70	K	1.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5396894&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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