Acetoacetic acid, benzyl ester

Other names:	Acetoacetic acid, benzyl ester
	Benzyl 3-oxobutanoate
	Benzyl acetoacetate
	Benzyl acetylacetate
	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:	38432-58-5

Physical Properties

Property code	Value	Unit	Source
hf	-422.73	kJ/mol	Cheméo Relay (1.0)
hfus	22.67	kJ/mol	Joback Method
hvap	68.39	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-1.74		Cheméo Relay (1.0)
logp	1.709		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
tb	541.55	K	Cheméo Relay (1.0)
tf	278.30	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.58	J/mol×K	607.92	Joback Method
cpg	376.71	J/mol×K	644.08	Joback Method
cpg	389.01	J/mol×K	680.23	Joback Method
cpg	400.49	J/mol×K	716.39	Joback Method
cpg	411.19	J/mol×K	752.55	Joback Method
cpg	421.12	J/mol×K	788.70	Joback Method

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	436.00	K	2.10	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38432585&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

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

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point