Ethyl benzoylacetate

Other names:	Benzenepropanoic acid, «beta»-oxo-, ethyl ester
	Acetic acid, benzoyl-, ethyl ester
	Benzoylacetic acid, ethyl ester
	Ethyl «beta»-oxobenzenepropanoate
Inchi:	InChI=1S/C11H12O3/c1-2-14-11(13)8-10(12)9-6-4-3-5-7-9/h3-7H,2,8H2,1H3
InchiKey:	GKKZMYDNDDMXSE-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	CCOC(=O)CC(=O)c1ccccc1
Mol. weight [g/mol]:	192.21
CAS:	94-02-0

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	-2.25		Crippen Method
logp	1.822		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	540.70	K	NIST Webbook
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	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
hvapt	72.10	kJ/mol	459.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C94020&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt: Enthalpy of vaporization at a given temperature
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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