BENZENEBUTANOIC ACID, .GAMMA.-OXO-, METHYL ESTER

Other names: Propionic acid, 3-benzoyl-, methyl ester
Methyl 3-benzoylpropionate
Methyl 3-benzoylpropanoate
Propionic acid, beta-benzoyl-, methyl ester

Inchi: InChI=1S/C11H12O3/c1-14-11(13)8-7-10(12)9-5-3-2-4-6-9/h2-6H,7-8H2,1H3

InchiKey: XVRCVKWYKYJEIG-UHFFFAOYSA-N

Formula: C11H12O3

SMILES: COC(=O)CCC(=O)c1ccccc1

Mol. weight [g/mol]: 192.21

Physical Properties

Property code	Value	Unit	Source
af	0.5614		Cheméo Relay (1.0)
gf	-208.69	kJ/mol	Joback Method
hf	-436.50	kJ/mol	Cheméo Relay (1.0)
hfus	22.67	kJ/mol	Joback Method
hvap	79.37	kJ/mol	Cheméo Relay (1.0)
ie	9.05	eV	Cheméo Relay (1.0)
log10ws	-2.16		Cheméo Relay (1.0)
logp	1.822		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	551.99	K	Cheméo Relay (1.0)
tc	752.32	K	Cheméo Relay (1.0)
tf	318.62	K	Cheméo Relay (1.0)
vc	0.554	m3/kmol	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	456.00 ± 2.00	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25333248&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):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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

ie:	Ionization energy
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