Benzoic acid, 2-benzoyl-, methyl ester

Other names:	2-Benzoylbenzoic acid, methyl ester
	Benzoic acid, o-benzoyl-, methyl ester
	Methyl o-benzoylbenzoate
	Methyl-2-benzoylbenzoate
	methyl 2-(benzoyl)benzoate
	o-(Methoxycarbonyl)benzophenone
	o-Benzoylbenzoic acid methyl ester
Inchi:	InChI=1S/C15H12O3/c1-18-15(17)13-10-6-5-9-12(13)14(16)11-7-3-2-4-8-11/h2-10H,1H3
InchiKey:	NQSMEZJWJJVYOI-UHFFFAOYSA-N
Formula:	C15H12O3
SMILES:	COC(=O)c1ccccc1C(=O)c1ccccc1
Mol. weight [g/mol]:	240.25
CAS:	606-28-0

Physical Properties

Property code	Value	Unit	Source
gf	-72.23	kJ/mol	Joback Method
hf	-248.72	kJ/mol	Joback Method
hfus	26.68	kJ/mol	Joback Method
hvap	70.10	kJ/mol	Joback Method
log10ws	-3.68		Aqueous Solubility Prediction Method
logp	2.704		Crippen Method
mcvol	183.700	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	625.00	K	NIST Webbook
tc	975.09	K	Joback Method
tf	325.00	K	NIST Webbook
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.02	J/mol×K	731.10	Joback Method

cpg	493.68	J/mol×K	771.76	Joback Method
cpg	506.15	J/mol×K	812.43	Joback Method
cpg	517.48	J/mol×K	853.09	Joback Method
cpg	527.71	J/mol×K	893.76	Joback Method
cpg	536.90	J/mol×K	934.42	Joback Method
cpg	545.09	J/mol×K	975.09	Joback Method
dvisc	0.0010757	Pa×s	446.26	Joback Method
dvisc	0.0006479	Pa×s	493.73	Joback Method
dvisc	0.0004265	Pa×s	541.21	Joback Method
dvisc	0.0003004	Pa×s	588.68	Joback Method
dvisc	0.0002229	Pa×s	636.15	Joback Method
dvisc	0.0001724	Pa×s	683.63	Joback Method
dvisc	0.0001379	Pa×s	731.10	Joback Method

Sources

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

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C606280&Units=SI

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

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume