Benzoic acid, 4-benzoyl-, methyl ester

Other names: Benzoic acid, p-benzoyl-, methyl ester
Methyl p-benzoyl benzoate
Methyl 4-benzophenonecarboxylate
Inchi: InChI=1S/C15H12O3/c1-18-15(17)13-9-7-12(8-10-13)14(16)11-5-3-2-4-6-11/h2-10H,1H3
InchiKey: UPXFXAMIFNGJLD-UHFFFAOYSA-N
Formula: C15H12O3
SMILES: COC(=O)c1ccc(C(=O)c2ccccc2)cc1
Mol. weight [g/mol]: 240.25
CAS: 6158-54-9

Physical Properties

Property code	Value	Unit	Source
ea	1.11 ± 0.09	eV	NIST Webbook
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	-3.67		Crippen Method
logp	2.704		Crippen Method
mcvol	183.700	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	731.10	K	Joback Method
tc	975.09	K	Joback Method
tf	446.26	K	Joback Method
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

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=C6158549&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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