Benzoylformic acid

Other names:	Phenylglyoxylic acid
	Benzeneacetic acid, «alpha»-oxo-
	«alpha»-Ketophenylacetic acid
	Benzeneglyoxylic acid
	Formic acid, benzoyl-
	Glyoxylic acid, phenyl-
	Oxophenylacetic acid
	Phenylgloxylic acid
	2-Oxo-2-phenylacetic acid
Inchi:	InChI=1S/C8H6O3/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5H,(H,10,11)
InchiKey:	FAQJJMHZNSSFSM-UHFFFAOYSA-N
Formula:	C8H6O3
SMILES:	O=C(O)C(=O)c1ccccc1
Mol. weight [g/mol]:	150.13
CAS:	611-73-4

Physical Properties

Property code	Value	Unit	Source
chs	-3518.35 ± 0.70	kJ/mol	NIST Webbook
gf	-265.77	kJ/mol	Joback Method
hf	-388.70 ± 1.00	kJ/mol	NIST Webbook
hfs	-487.22 ± 0.80	kJ/mol	NIST Webbook
hfus	17.80	kJ/mol	Joback Method
hsub	98.50	kJ/mol	NIST Webbook
hvap	65.85	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.954		Crippen Method
mcvol	108.830	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
tb	609.04	K	Joback Method
tc	823.00	K	Joback Method
tf	338.90 ± 0.50	K	NIST Webbook
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.74	J/mol×K	609.04	Joback Method
cpg	288.67	J/mol×K	823.00	Joback Method
cpg	283.02	J/mol×K	787.34	Joback Method
cpg	276.87	J/mol×K	751.68	Joback Method
cpg	270.20	J/mol×K	716.02	Joback Method
cpg	262.97	J/mol×K	680.36	Joback Method
cpg	255.16	J/mol×K	644.70	Joback Method
cps	192.90	J/mol×K	298.15	NIST Webbook
dvisc	0.0016252	Pa×s	407.36	Joback Method
dvisc	0.0001103	Pa×s	609.04	Joback Method
dvisc	0.0001622	Pa×s	568.70	Joback Method
dvisc	0.0002529	Pa×s	528.37	Joback Method
dvisc	0.0004244	Pa×s	488.03	Joback Method
dvisc	0.0007817	Pa×s	447.69	Joback Method
dvisc	0.0039687	Pa×s	367.02	Joback Method
hfust	21.80	kJ/mol	338.90	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C611734&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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