Phenylglyoxal

Other names:	Benzeneacetaldehyde, «alpha»-oxo-
	Glyoxal, phenyl-
	Benzoylcarboxaldehyde
	Benzoylformaldehyde
	Phenylethanedione
Inchi:	InChI=1S/C8H6O2/c9-6-8(10)7-4-2-1-3-5-7/h1-6H
InchiKey:	OJUGVDODNPJEEC-UHFFFAOYSA-N
Formula:	C8H6O2
SMILES:	O=CC(=O)c1ccccc1
Mol. weight [g/mol]:	134.13
CAS:	1074-12-0

Physical Properties

Property code	Value	Unit	Source
gf	-99.55	kJ/mol	Joback Method
hf	-170.08	kJ/mol	Joback Method
hfus	14.40	kJ/mol	Joback Method
hvap	49.14	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.068		Crippen Method
mcvol	102.960	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	511.65	K	Joback Method
tc	737.89	K	Joback Method
tf	298.27	K	Joback Method
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.90	J/mol×K	737.89	Joback Method
cpg	251.94	J/mol×K	700.18	Joback Method
cpg	244.39	J/mol×K	662.48	Joback Method
cpg	236.21	J/mol×K	624.77	Joback Method

cpg	227.36	J/mol×K	587.06	Joback Method
cpg	217.82	J/mol×K	549.36	Joback Method
cpg	207.56	J/mol×K	511.65	Joback Method
dvisc	0.0029837	Pa×s	298.27	Joback Method
dvisc	0.0003484	Pa×s	511.65	Joback Method
dvisc	0.0004360	Pa×s	476.09	Joback Method
dvisc	0.0005657	Pa×s	440.52	Joback Method
dvisc	0.0007683	Pa×s	404.96	Joback Method
dvisc	0.0011070	Pa×s	369.40	Joback Method
dvisc	0.0017239	Pa×s	333.83	Joback Method
hvapt	59.70	kJ/mol	407.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.20	K	16.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1074120&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume