Ethanone, 1,1'-(1,3-phenylene)bis-

Other names:	1,3-Diacetylbenzene
	m-Diacetylbenzene
	m-Acetyl acetophenone
	3-CH3CO-C6H4-COCH3
	benzene-1,3-bis(acetyl)
Inchi:	InChI=1S/C10H10O2/c1-7(11)9-4-3-5-10(6-9)8(2)12/h3-6H,1-2H3
InchiKey:	VCHOFVSNWYPAEF-UHFFFAOYSA-N
Formula:	C10H10O2
SMILES:	CC(=O)c1cccc(C(C)=O)c1
Mol. weight [g/mol]:	162.19
CAS:	6781-42-6

Physical Properties

Property code	Value	Unit	Source
affp	852.00	kJ/mol	NIST Webbook
basg	822.30	kJ/mol	NIST Webbook
gf	-121.74	kJ/mol	Joback Method
hf	-249.83	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	54.28	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.092		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
ripol	2333.00		NIST Webbook
tb	567.60	K	Joback Method
tc	792.32	K	Joback Method
tf	341.26	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.49	J/mol×K	567.60	Joback Method

cpg	304.79	J/mol×K	605.05	Joback Method
cpg	316.30	J/mol×K	642.51	Joback Method
cpg	327.04	J/mol×K	679.96	Joback Method
cpg	337.05	J/mol×K	717.41	Joback Method
cpg	346.35	J/mol×K	754.86	Joback Method
cpg	354.96	J/mol×K	792.32	Joback Method
dvisc	0.0020791	Pa×s	341.26	Joback Method
dvisc	0.0012565	Pa×s	378.98	Joback Method
dvisc	0.0008319	Pa×s	416.71	Joback Method
dvisc	0.0005898	Pa×s	454.43	Joback Method
dvisc	0.0004408	Pa×s	492.15	Joback Method
dvisc	0.0003433	Pa×s	529.88	Joback Method
dvisc	0.0002765	Pa×s	567.60	Joback Method
hvapt	43.20	kJ/mol	370.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	425.70	K	2.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6781426&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity
basg: Gas basicity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume