3-hydroxy-4-phenyl-3-buten-2-one

Inchi: InChI=1S/C10H10O2/c1-8(11)10(12)7-9-5-3-2-4-6-9/h2-7,12H,1H3/b10-7-
InchiKey: FXMXAFDOFYLVFW-YFHOEESVSA-N
Formula: C10H10O2
SMILES: CC(=O)C(O)=Cc1ccccc1
Mol. weight [g/mol]: 162.19

Physical Properties

Property code	Value	Unit	Source
gf	-48.34	kJ/mol	Joback Method
hf	-170.58	kJ/mol	Joback Method
hfus	20.28	kJ/mol	Joback Method
hvap	63.59	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.174		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	1433.00		NIST Webbook
tb	604.97	K	Joback Method
tc	817.08	K	Joback Method
tf	320.59	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.62	J/mol×K	604.97	Joback Method
cpg	317.42	J/mol×K	640.32	Joback Method
cpg	327.48	J/mol×K	675.67	Joback Method
cpg	336.84	J/mol×K	711.02	Joback Method
cpg	345.56	J/mol×K	746.37	Joback Method
cpg	353.69	J/mol×K	781.72	Joback Method
cpg	361.26	J/mol×K	817.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515914&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume