o-Acetoacetylphenol

Other names: o-Hydroxybenzoylacetone
Inchi: InChI=1S/C10H10O3/c1-7(11)6-10(13)8-4-2-3-5-9(8)12/h2-5,12H,6H2,1H3
InchiKey: FAIACLOKYTYHSR-UHFFFAOYSA-N
Formula: C10H10O3
SMILES: CC(=O)CC(=O)c1ccccc1O
Mol. weight [g/mol]: 178.18
CAS: 16636-62-7

Physical Properties

Property code	Value	Unit	Source
gf	-266.73	kJ/mol	Joback Method
hf	-415.67	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	66.64	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.554		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	643.24	K	Joback Method
tc	876.58	K	Joback Method
tf	440.46	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.24	J/mol×K	643.24	Joback Method
cpg	386.59	J/mol×K	837.69	Joback Method
cpg	378.36	J/mol×K	798.80	Joback Method
cpg	369.59	J/mol×K	759.91	Joback Method
cpg	360.21	J/mol×K	721.02	Joback Method
cpg	350.12	J/mol×K	682.13	Joback Method
cpg	394.38	J/mol×K	876.58	Joback Method
dvisc	0.0000348	Pa×s	643.24	Joback Method

dvisc	0.0000504	Pa×s	609.44	Joback Method
dvisc	0.0000762	Pa×s	575.65	Joback Method
dvisc	0.0001214	Pa×s	541.85	Joback Method
dvisc	0.0002055	Pa×s	508.05	Joback Method
dvisc	0.0003752	Pa×s	474.26	Joback Method
dvisc	0.0007511	Pa×s	440.46	Joback Method

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=C16636627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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