Benzoic acid, 2-(1-oxopropyl)-

Other names: 2-(1-oxopropyl)benzoic acid
Inchi: InChI=1S/C10H10O3/c1-2-9(11)7-5-3-4-6-8(7)10(12)13/h3-6H,2H2,1H3,(H,12,13)
InchiKey: JYBOOAWVGOYQFU-UHFFFAOYSA-N
Formula: C10H10O3
SMILES: CCC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 178.18
CAS: 2360-45-4

Physical Properties

Property code	Value	Unit	Source
gf	-258.56	kJ/mol	Joback Method
hf	-402.06	kJ/mol	Joback Method
hfus	22.59	kJ/mol	Joback Method
hvap	70.96	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.978		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	659.78	K	Joback Method
tc	867.95	K	Joback Method
tf	402.08	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.64	J/mol×K	659.78	Joback Method
cpg	381.81	J/mol×K	833.25	Joback Method
cpg	374.37	J/mol×K	798.56	Joback Method
cpg	366.36	J/mol×K	763.86	Joback Method
cpg	357.75	J/mol×K	729.17	Joback Method
cpg	348.52	J/mol×K	694.47	Joback Method
cpg	388.70	J/mol×K	867.95	Joback Method
dvisc	0.0000783	Pa×s	659.78	Joback Method

dvisc	0.0001126	Pa×s	616.83	Joback Method
dvisc	0.0001711	Pa×s	573.88	Joback Method
dvisc	0.0002782	Pa×s	530.93	Joback Method
dvisc	0.0004925	Pa×s	487.98	Joback Method
dvisc	0.0009736	Pa×s	445.03	Joback Method
dvisc	0.0022265	Pa×s	402.08	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=C2360454&Units=SI

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