Benzoic acid, 3-hydroxy-, 1-methylethyl ester

Other names:	Benzoic acid, 3-hydroxy-, isopropyl ester
	Isopropyl 3-hydroxybenzoate
Inchi:	InChI=1S/C10H12O3/c1-7(2)13-10(12)8-4-3-5-9(11)6-8/h3-7,11H,1-2H3
InchiKey:	VANDBVAFPVUVNX-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	CC(C)OC(=O)c1cccc(O)c1
Mol. weight [g/mol]:	180.20
CAS:	53631-77-9

Physical Properties

Property code	Value	Unit	Source
gf	-245.25	kJ/mol	Joback Method
hf	-440.59	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	61.91	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.957		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
rinpol	1501.00		NIST Webbook
tb	611.35	K	Joback Method
tc	839.56	K	Joback Method
tf	397.76	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.96	J/mol×K	611.35	Joback Method
cpg	363.37	J/mol×K	649.38	Joback Method
cpg	374.95	J/mol×K	687.42	Joback Method
cpg	385.76	J/mol×K	725.45	Joback Method
cpg	395.88	J/mol×K	763.49	Joback Method
cpg	405.36	J/mol×K	801.52	Joback Method

cpg	414.28	J/mol×K	839.56	Joback Method
dvisc	0.0012031	Pa×s	397.76	Joback Method
dvisc	0.0005049	Pa×s	433.36	Joback Method
dvisc	0.0002417	Pa×s	468.96	Joback Method
dvisc	0.0001284	Pa×s	504.56	Joback Method
dvisc	0.0000742	Pa×s	540.15	Joback Method
dvisc	0.0000458	Pa×s	575.75	Joback Method
dvisc	0.0000300	Pa×s	611.35	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=C53631779&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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