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

Physical Properties

Property code	Value	Unit	Source
hf	-513.22	kJ/mol	Cheméo Relay (1.0)
hfus	20.74	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Cheméo Relay (1.0)
ie	8.68	eV	Cheméo Relay (1.0)
logp	1.957		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
rinpol	1501.00		NIST Webbook
tb	541.47	K	Cheméo Relay (1.0)
tc	745.51	K	Cheméo Relay (1.0)
tf	343.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.96	J/mol×K	611.35	Joback Method
cpg	414.28	J/mol×K	839.56	Joback Method
cpg	405.36	J/mol×K	801.52	Joback Method
cpg	395.88	J/mol×K	763.49	Joback Method
cpg	385.76	J/mol×K	725.45	Joback Method
cpg	374.95	J/mol×K	687.42	Joback Method
cpg	363.37	J/mol×K	649.38	Joback Method
dvisc	0.0001284	Pa×s	504.56	Joback Method
dvisc	0.0000300	Pa×s	611.35	Joback Method

dvisc	0.0000458	Pa×s	575.75	Joback Method
dvisc	0.0000742	Pa×s	540.15	Joback Method
dvisc	0.0012031	Pa×s	397.76	Joback Method
dvisc	0.0002417	Pa×s	468.96	Joback Method
dvisc	0.0005049	Pa×s	433.36	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53631779&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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