ISOPROPYL P-HYDROXYBENZOATE

Inchi: InChI=1S/C10H12O3/c1-7(2)13-10(12)8-3-5-9(11)6-4-8/h3-7,11H,1-2H3
InchiKey: CMHMMKSPYOOVGI-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: CC(C)OC(=O)c1ccc(O)cc1
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
hf	-519.24	kJ/mol	Cheméo Relay (1.0)
hfus	20.74	kJ/mol	Joback Method
hvap	77.74	kJ/mol	Cheméo Relay (1.0)
ie	8.61	eV	Cheméo Relay (1.0)
log10ws	-2.17		Cheméo Relay (1.0)
logp	1.957		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
tb	543.85	K	Cheméo Relay (1.0)
tf	371.86	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

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=C4191735&Units=SI
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point