

isopropyl 4-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
CAS:	4191-73-5

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
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/molxK	611.35	Joback Method
cpg	363.37	J/molxK	649.38	Joback Method
cpg	374.95	J/molxK	687.42	Joback Method
cpg	385.76	J/molxK	725.45	Joback Method
cpg	395.88	J/molxK	763.49	Joback Method
cpg	405.36	J/molxK	801.52	Joback Method
cpg	414.28	J/molxK	839.56	Joback Method
dvisc	0.0012031	Paxs	397.76	Joback Method
dvisc	0.0005049	Paxs	433.36	Joback Method

dvisc	0.0002417	Paxs	468.96	Joback Method
dvisc	0.0001284	Paxs	504.56	Joback Method
dvisc	0.0000742	Paxs	540.15	Joback Method
dvisc	0.0000458	Paxs	575.75	Joback Method
dvisc	0.0000300	Paxs	611.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4191735&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

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