2-(Isopropoxycarbonyl)benzoic acid

Inchi: InChI=1S/C11H12O4/c1-7(2)15-11(14)9-6-4-3-5-8(9)10(12)13/h3-7H,1-2H3,(H,12,13)
InchiKey: CXJOEMLCEGZVPL-UHFFFAOYSA-N
Formula: C11H12O4
SMILES: CC(C)OC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 208.21
CAS: 35118-50-4

Physical Properties

Property code	Value	Unit	Source
gf	-357.58	kJ/mol	Joback Method
hf	-560.20	kJ/mol	Joback Method
hfus	22.85	kJ/mol	Joback Method
hvap	75.21	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	1.950		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
rinpol	1667.00		NIST Webbook
rinpol	1667.00		NIST Webbook
tb	704.64	K	Joback Method
tc	911.71	K	Joback Method
tf	420.58	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.11	J/mol×K	704.64	Joback Method
cpg	422.73	J/mol×K	739.15	Joback Method
cpg	432.64	J/mol×K	773.66	Joback Method
cpg	441.85	J/mol×K	808.18	Joback Method
cpg	450.38	J/mol×K	842.69	Joback Method
cpg	458.24	J/mol×K	877.20	Joback Method
cpg	465.45	J/mol×K	911.71	Joback Method

dvisc	0.0015908	Pa×s	420.58	Joback Method
dvisc	0.0006532	Pa×s	467.92	Joback Method
dvisc	0.0003159	Pa×s	515.27	Joback Method
dvisc	0.0001726	Pa×s	562.61	Joback Method
dvisc	0.0001036	Pa×s	609.95	Joback Method
dvisc	0.0000669	Pa×s	657.30	Joback Method
dvisc	0.0000458	Pa×s	704.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35118504&Units=SI
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

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