Benzoic acid, 1-methylethyl ester

Other names:	Benzoic acid, isopropyl ester
	Isopropyl benzoate
	Isopropylester kyseliny benzoove
Inchi:	InChI=1S/C10H12O2/c1-8(2)12-10(11)9-6-4-3-5-7-9/h3-8H,1-2H3
InchiKey:	FEXQDZTYJVXMOS-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC(C)OC(=O)c1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	939-48-0

Physical Properties

Property code	Value	Unit	Source
gf	-90.63	kJ/mol	Joback Method
hf	-263.28	kJ/mol	Joback Method
hfus	14.96	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.252		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	1212.70		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1207.20		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1216.70		NIST Webbook
rinpol	1219.70		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1193.00		NIST Webbook

rinpol	1223.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1219.70		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1223.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1639.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1676.00		NIST Webbook
tb	491.65 ± 1.00	K	NIST Webbook
tb	491.50 ± 0.50	K	NIST Webbook
tb	491.00	K	NIST Webbook
tb	491.20	K	NIST Webbook
tc	748.19	K	Joback Method
tf	286.04	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.78	J/mol×K	530.73	Joback Method
cpg	314.76	J/mol×K	566.97	Joback Method
cpg	327.92	J/mol×K	603.22	Joback Method
cpg	340.30	J/mol×K	639.46	Joback Method
cpg	351.91	J/mol×K	675.70	Joback Method
cpg	362.77	J/mol×K	711.95	Joback Method
cpg	372.90	J/mol×K	748.19	Joback Method
dvisc	0.0031130	Pa×s	286.04	Joback Method
dvisc	0.0014883	Pa×s	326.82	Joback Method
dvisc	0.0008382	Pa×s	367.60	Joback Method
dvisc	0.0005294	Pa×s	408.38	Joback Method

dvisc	0.0003634	Pa×s	449.17	Joback Method
dvisc	0.0002656	Pa×s	489.95	Joback Method
dvisc	0.0002037	Pa×s	530.73	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=C939480&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume