Benzoic acid, 1-methylpropyl ester

Other names:	1-Methylpropyl benzoate
	Sec-butyl benzoate
Inchi:	InChI=1S/C11H14O2/c1-3-9(2)13-11(12)10-7-5-4-6-8-10/h4-9H,3H2,1-2H3
InchiKey:	LSLWNAOQPPLHSW-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCC(C)OC(=O)c1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	3306-36-3

Physical Properties

Property code	Value	Unit	Source
gf	-82.21	kJ/mol	Joback Method
hf	-283.92	kJ/mol	Joback Method
hfus	17.55	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.642		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1288.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1766.00		NIST Webbook

ripol	1774.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1749.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1752.00		NIST Webbook
tb	553.61	K	Joback Method
tc	767.42	K	Joback Method
tf	297.31	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.73	J/mol×K	553.61	Joback Method
cpg	412.55	J/mol×K	731.79	Joback Method
cpg	401.00	J/mol×K	696.15	Joback Method
cpg	388.67	J/mol×K	660.52	Joback Method
cpg	375.53	J/mol×K	624.88	Joback Method
cpg	361.56	J/mol×K	589.25	Joback Method
cpg	423.32	J/mol×K	767.42	Joback Method
dvisc	0.0001883	Pa×s	553.61	Joback Method
dvisc	0.0002466	Pa×s	510.89	Joback Method
dvisc	0.0003393	Pa×s	468.18	Joback Method
dvisc	0.0004976	Pa×s	425.46	Joback Method
dvisc	0.0007949	Pa×s	382.74	Joback Method
dvisc	0.0014284	Pa×s	340.03	Joback Method
dvisc	0.0030377	Pa×s	297.31	Joback Method

Sources

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=C3306363&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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