Benzoic acid, 2-methoxy-, tert.-butyl ester

Inchi: InChI=1S/C12H16O3/c1-12(2,3)15-11(13)9-7-5-6-8-10(9)14-4/h5-8H,1-4H3
InchiKey: BQFFOUQBTAMINL-UHFFFAOYSA-N
Formula: C12H16O3
SMILES: COc1ccccc1C(=O)OC(C)(C)C
Mol. weight [g/mol]: 208.25

Physical Properties

Property code	Value	Unit	Source
gf	-183.14	kJ/mol	Joback Method
hf	-451.72	kJ/mol	Joback Method
hfus	17.05	kJ/mol	Joback Method
hvap	55.51	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.651		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook
tb	601.10	K	Joback Method
tc	818.07	K	Joback Method
tf	360.75	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.60	J/mol×K	601.10	Joback Method
cpg	438.00	J/mol×K	637.26	Joback Method
cpg	452.46	J/mol×K	673.42	Joback Method
cpg	466.00	J/mol×K	709.58	Joback Method
cpg	478.65	J/mol×K	745.74	Joback Method
cpg	490.42	J/mol×K	781.91	Joback Method
cpg	501.35	J/mol×K	818.07	Joback Method
dvisc	0.0014033	Pa×s	360.75	Joback Method

dvisc	0.0007728	Pa×s	400.81	Joback Method
dvisc	0.0004743	Pa×s	440.87	Joback Method
dvisc	0.0003158	Pa×s	480.92	Joback Method
dvisc	0.0002238	Pa×s	520.98	Joback Method
dvisc	0.0001666	Pa×s	561.04	Joback Method
dvisc	0.0001290	Pa×s	601.10	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=U375393&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume