2-Methoxyphenyl benzoate

Other names:	o-Methoxyphenyl benzoate
	Phenol, 2-methoxy-, benzoate
	o-Anisyl benzoate
	Benzcaine
	Benzosol
	Benzoylguaiacol
	Guaiacol benzoate
	Phenol, o-methoxy-, benzoate
	2-Methyoxyphenyl benzoate
	Benzoguaiacol
	Benzoic acid, 2-methoxyphenyl ester
Inchi:	InChI=1S/C14H12O3/c1-16-12-9-5-6-10-13(12)17-14(15)11-7-3-2-4-8-11/h2-10H,1H3
InchiKey:	IZYQCDNLUPLXOO-UHFFFAOYSA-N
Formula:	C14H12O3
SMILES:	COc1ccccc1OC(=O)c1ccccc1
Mol. weight [g/mol]:	228.24
CAS:	531-37-3

Physical Properties

Property code	Value	Unit	Source
gf	-56.73	kJ/mol	Joback Method
hf	-247.72	kJ/mol	Joback Method
hfus	23.68	kJ/mol	Joback Method
hvap	63.54	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	2.914		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1893.00		NIST Webbook
rinpol	1893.00		NIST Webbook
tb	676.77	K	Joback Method
tc	916.60	K	Joback Method
tf	407.29	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.07	J/mol×K	676.77	Joback Method
cpg	454.76	J/mol×K	716.74	Joback Method
cpg	468.31	J/mol×K	756.71	Joback Method
cpg	480.73	J/mol×K	796.68	Joback Method
cpg	492.07	J/mol×K	836.66	Joback Method
cpg	502.33	J/mol×K	876.63	Joback Method
cpg	511.55	J/mol×K	916.60	Joback Method
dvisc	0.0009553	Pa×s	407.29	Joback Method
dvisc	0.0005676	Pa×s	452.20	Joback Method
dvisc	0.0003705	Pa×s	497.12	Joback Method
dvisc	0.0002596	Pa×s	542.03	Joback Method
dvisc	0.0001921	Pa×s	586.94	Joback Method
dvisc	0.0001483	Pa×s	631.86	Joback Method
dvisc	0.0001185	Pa×s	676.77	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=C531373&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