

Benzoic acid, 2-methoxy-, phenyl ester

Other names:	o-Methoxybenzoic acid, phenyl ester
Inchi:	InChI=1S/C14H12O3/c1-16-13-10-6-5-9-12(13)14(15)17-11-7-3-2-4-8-11/h2-10H,1H3
InchiKey:	LZRFQYZCMVMADF-UHFFFAOYSA-N
Formula:	C14H12O3
SMILES:	COc1ccccc1C(=O)Oc1ccccc1
Mol. weight [g/mol]:	228.24
CAS:	10268-71-0

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	1859.40		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	502.33	J/mol×K	876.63	Joback Method
cpg	492.07	J/mol×K	836.66	Joback Method
cpg	480.73	J/mol×K	796.68	Joback Method
cpg	468.31	J/mol×K	756.71	Joback Method
cpg	454.76	J/mol×K	716.74	Joback Method
cpg	511.55	J/mol×K	916.60	Joback Method

dvisc	0.0001185	Pa×s	676.77	Joback Method
dvisc	0.0001483	Pa×s	631.86	Joback Method
dvisc	0.0001921	Pa×s	586.94	Joback Method
dvisc	0.0002596	Pa×s	542.03	Joback Method
dvisc	0.0003705	Pa×s	497.12	Joback Method
dvisc	0.0005676	Pa×s	452.20	Joback Method
dvisc	0.0009553	Pa×s	407.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10268710&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

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