Benzoic acid, 4-methoxy-, phenyl ester

Other names: p-Methoxybenzoic acid, phenyl ester
Inchi: InChI=1S/C14H12O3/c1-16-12-9-7-11(8-10-12)14(15)17-13-5-3-2-4-6-13/h2-10H,1H3
InchiKey: BNZYBNYNPXKWCM-UHFFFAOYSA-N
Formula: C14H12O3
SMILES: COc1ccc(C(=O)Oc2ccccc2)cc1
Mol. weight [g/mol]: 228.24
CAS: 4181-97-9

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	1905.90		NIST Webbook
rinpol	1905.90		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: 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=C4181979&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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