Benzoic acid, 4-methylphenyl ester

Other names:	p-Tolyl benzoate
	Benzoic acid, p-tolyl ester
	4-Methylphenyl benzoate
	p-Cresyl benzoate
	Benzoic acid, 4-tolyl ester
Inchi:	InChI=1S/C14H12O2/c1-11-7-9-13(10-8-11)16-14(15)12-5-3-2-4-6-12/h2-10H,1H3
InchiKey:	LLRZUDIHEZXFGV-UHFFFAOYSA-N
Formula:	C14H12O2
SMILES:	Cc1ccc(OC(=O)c2ccccc2)cc1
Mol. weight [g/mol]:	212.24
CAS:	614-34-6

Physical Properties

Property code	Value	Unit	Source
gf	48.27	kJ/mol	Joback Method
hf	-115.50	kJ/mol	Joback Method
hfus	22.50	kJ/mol	Joback Method
hvap	61.13	kJ/mol	Joback Method
ie	8.27	eV	NIST Webbook
log10ws	-4.03		Crippen Method
logp	3.214		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1764.00		NIST Webbook
rinpol	1764.00		NIST Webbook
tb	654.35	K	Joback Method
tc	898.02	K	Joback Method
tf	385.06	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.01	J/mol×K	654.35	Joback Method

cpg	479.16	J/mol×K	857.41	Joback Method
cpg	468.50	J/mol×K	816.80	Joback Method
cpg	456.81	J/mol×K	776.19	Joback Method
cpg	444.02	J/mol×K	735.57	Joback Method
cpg	430.11	J/mol×K	694.96	Joback Method
cpg	488.82	J/mol×K	898.02	Joback Method
dvisc	0.0001499	Pa×s	654.35	Joback Method
dvisc	0.0001880	Pa×s	609.47	Joback Method
dvisc	0.0002444	Pa×s	564.59	Joback Method
dvisc	0.0003325	Pa×s	519.71	Joback Method
dvisc	0.0004795	Pa×s	474.82	Joback Method
dvisc	0.0007464	Pa×s	429.94	Joback Method
dvisc	0.0012880	Pa×s	385.06	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=C614346&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
ie: Ionization energy
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