Benzoic acid, 2-(4-methylbenzoyl)-

Other names:	Benzoic acid, o-(p-toluoyl)-
	o-(p-Toluoyl)benzoic acid
	2-(p-Toluyl)benzoic acid
	2-(4-Methylbenzoyl)benzoic acid
	4'-Methylbenzophenone-2-carboxylic acid
	2-(p-Toluoyl)benzoic acid
	p-Toluoyl-o-benzoic acid
Inchi:	InChI=1S/C15H12O3/c1-10-6-8-11(9-7-10)14(16)12-4-2-3-5-13(12)15(17)18/h2-9H,1H3,(
InchiKey:	ICQOWIXIHDDXDI-UHFFFAOYSA-N
Formula:	C15H12O3
SMILES:	Cc1ccc(C(=O)c2ccccc2C(=O)O)cc1
Mol. weight [g/mol]:	240.25
CAS:	85-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-113.68	kJ/mol	Joback Method
hf	-280.20	kJ/mol	Joback Method
hfus	29.20	kJ/mol	Joback Method
hvap	85.03	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	2.924		Crippen Method
mcvol	183.700	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	805.84	K	Joback Method
tc	1035.00	K	Joback Method
tf	497.37	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.16	J/mol×K	805.84	Joback Method
cpg	546.18	J/mol×K	996.81	Joback Method

cpg	538.76	J/mol×K	958.62	Joback Method
cpg	530.60	J/mol×K	920.42	Joback Method
cpg	521.65	J/mol×K	882.23	Joback Method
cpg	511.86	J/mol×K	844.03	Joback Method
cpg	552.92	J/mol×K	1035.00	Joback Method
dvisc	0.0000328	Pa×s	805.84	Joback Method
dvisc	0.0000456	Pa×s	754.43	Joback Method
dvisc	0.0000665	Pa×s	703.02	Joback Method
dvisc	0.0001030	Pa×s	651.61	Joback Method
dvisc	0.0001720	Pa×s	600.19	Joback Method
dvisc	0.0003162	Pa×s	548.78	Joback Method
dvisc	0.0006590	Pa×s	497.37	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=C85552&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume