

Benzoic acid, 2-hydroxy-, 4-methylphenyl ester

Other names:	p-Cresyl salicylate p-Tolyl salicylate Salicylic acid, p-tolyl ester 4-Methylphenyl salicylate 4-Methylphenyl 2-hydroxybenzoate
Inchi:	InChI=1S/C14H12O3/c1-10-6-8-11(9-7-10)17-14(16)12-4-2-3-5-13(12)15/h2-9,15H,1H3
InchiKey:	AMYKXJAXRJCLCV-UHFFFAOYSA-N
Formula:	C14H12O3
SMILES:	Cc1ccc(OC(=O)c2ccccc2O)cc1
Mol. weight [g/mol]:	228.24
CAS:	607-88-5

Physical Properties

Property code	Value	Unit	Source
gf	-106.35	kJ/mol	Joback Method
hf	-292.81	kJ/mol	Joback Method
hfus	28.28	kJ/mol	Joback Method
hvap	74.14	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.920		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	1850.00		NIST Webbook
tb	734.97	K	Joback Method
tc	985.71	K	Joback Method
tf	496.78	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.89	J/mol×K	734.97	Joback Method
cpg	475.85	J/mol×K	776.76	Joback Method
cpg	487.84	J/mol×K	818.55	Joback Method

cpg	498.98	J/mol×K	860.34	Joback Method
cpg	509.38	J/mol×K	902.13	Joback Method
cpg	519.15	J/mol×K	943.92	Joback Method
cpg	528.39	J/mol×K	985.71	Joback Method
dvisc	0.0002250	Pa×s	496.78	Joback Method
dvisc	0.0001147	Pa×s	536.48	Joback Method
dvisc	0.0000641	Pa×s	576.18	Joback Method
dvisc	0.0000387	Pa×s	615.88	Joback Method
dvisc	0.0000248	Pa×s	655.57	Joback Method
dvisc	0.0000167	Pa×s	695.27	Joback Method
dvisc	0.0000118	Pa×s	734.97	Joback Method

Sources

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=C607885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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