p-tert-Butylphenylsalicylate

Other names:	4-tert-Butylphenyl salicylate
	Salicylic acid p-tert-butylphenyl ester
	Benzoic acid, 2-hydroxy-, 4-(1,1-dimethylethyl)phenyl ester
	Salicyclic acid p-tert-butylphenyl ester
	UV Absorber NL/3
	p-terc.Butylfenylester kyseliny salicylove
	4-(t-Butylphenyl) salicyclate
	Salicyclic acid, 4-(t-butylphenyl) ester
Inchi:	InChI=1S/C17H18O3/c1-17(2,3)12-8-10-13(11-9-12)20-16(19)14-6-4-5-7-15(14)18/h4-11
InchiKey:	DBOSBRHMHBENLP-UHFFFAOYSA-N
Formula:	C17H18O3
SMILES:	CC(C)(C)c1ccc(OC(=O)c2ccccc2O)cc1
Mol. weight [g/mol]:	270.32
CAS:	87-18-3

Physical Properties

Property code	Value	Unit	Source
gf	-78.25	kJ/mol	Joback Method
hf	-363.48	kJ/mol	Joback Method
hfus	28.64	kJ/mol	Joback Method
hvap	79.52	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.909		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
tb	800.38	K	Joback Method
tc	1048.95	K	Joback Method
tf	533.01	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.97	J/mol×K	1048.95	Joback Method

cpg	624.93	J/mol×K	800.38	Joback Method
cpg	639.58	J/mol×K	841.81	Joback Method
cpg	653.24	J/mol×K	883.24	Joback Method
cpg	666.05	J/mol×K	924.67	Joback Method
cpg	678.17	J/mol×K	966.09	Joback Method
cpg	689.76	J/mol×K	1007.52	Joback Method
dvisc	0.0000052	Pa×s	800.38	Joback Method
dvisc	0.0001235	Pa×s	533.01	Joback Method
dvisc	0.0000595	Pa×s	577.57	Joback Method
dvisc	0.0000318	Pa×s	622.13	Joback Method
dvisc	0.0000185	Pa×s	666.69	Joback Method
dvisc	0.0000115	Pa×s	711.26	Joback Method
dvisc	0.0000076	Pa×s	755.82	Joback Method
hsubt	137.40	kJ/mol	314.50	NIST Webbook
hvapt	90.40	kJ/mol	387.00	NIST Webbook

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=C87183&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
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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

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