Benzoic acid, 2-hydroxy-, pentyl ester

Other names:	Salicylic acid, pentyl ester
	Amyl salicylate
	Pentyl salicylate
	Amylester kyseliny salicylove
	N-Amyl salicylate
	Salicylic acid, amyl ester
Inchi:	InChI=1S/C12H16O3/c1-2-3-6-9-15-12(14)10-7-4-5-8-11(10)13/h4-5,7-8,13H,2-3,6,9H2,1
InchiKey:	RANVDUNFZBMTBK-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	CCCCCOC(=O)c1ccccc1O
Mol. weight [g/mol]:	208.25
CAS:	2050-08-0

Physical Properties

Property code	Value	Unit	Source
gf	-225.97	kJ/mol	Joback Method
hf	-476.59	kJ/mol	Joback Method
hfus	29.45	kJ/mol	Joback Method
hvap	66.75	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.739		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	1552.00		NIST Webbook
rinpol	1552.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1535.00		NIST Webbook
ripol	2077.00		NIST Webbook
ripol	2055.00		NIST Webbook
ripol	2066.00		NIST Webbook
ripol	2077.00		NIST Webbook
ripol	2097.00		NIST Webbook

ripol	2093.00		NIST Webbook
tb	657.55	K	Joback Method
tc	873.24	K	Joback Method
tf	435.30	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.08	J/mol×K	657.55	Joback Method
cpg	461.57	J/mol×K	693.50	Joback Method
cpg	474.24	J/mol×K	729.45	Joback Method
cpg	486.16	J/mol×K	765.40	Joback Method
cpg	497.38	J/mol×K	801.34	Joback Method
cpg	507.98	J/mol×K	837.29	Joback Method
cpg	518.02	J/mol×K	873.24	Joback Method
dvisc	0.0006064	Pa×s	435.30	Joback Method
dvisc	0.0002767	Pa×s	472.34	Joback Method
dvisc	0.0001415	Pa×s	509.38	Joback Method
dvisc	0.0000793	Pa×s	546.42	Joback Method
dvisc	0.0000478	Pa×s	583.47	Joback Method
dvisc	0.0000306	Pa×s	620.51	Joback Method
dvisc	0.0000206	Pa×s	657.55	Joback Method
hvapt	66.50	kJ/mol	471.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050080&Units=SI

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

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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume