Benzoic acid, 2-hydroxy-, propyl ester

Other names:	Propyl o-hydroxybenzoate
	Propyl salicylate
	Salicylic acid, propyl ester
	Salicylic acid, n-propyl ester
	n-Propyl salicylate
Inchi:	InChI=1S/C10H12O3/c1-2-7-13-10(12)8-5-3-4-6-9(8)11/h3-6,11H,2,7H2,1H3
InchiKey:	LZFIOSVZIQOVFW-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	CCCOC(=O)c1ccccc1O
Mol. weight [g/mol]:	180.20
CAS:	607-90-9

Physical Properties

Property code	Value	Unit	Source
gf	-242.81	kJ/mol	Joback Method
hf	-435.31	kJ/mol	Joback Method
hfus	24.27	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.959		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
rinpol	1357.00		NIST Webbook
rinpol	1385.00		NIST Webbook
ripol	1878.00		NIST Webbook
tb	611.79	K	Joback Method
tc	835.24	K	Joback Method
tf	412.76	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.48	J/mol×K	611.79	Joback Method

cpg	362.58	J/mol×K	649.03	Joback Method
cpg	373.90	J/mol×K	686.27	Joback Method
cpg	384.49	J/mol×K	723.51	Joback Method
cpg	394.42	J/mol×K	760.76	Joback Method
cpg	403.75	J/mol×K	798.00	Joback Method
cpg	412.55	J/mol×K	835.24	Joback Method
dvisc	0.0008548	Pa×s	412.76	Joback Method
dvisc	0.0004034	Pa×s	445.93	Joback Method
dvisc	0.0002113	Pa×s	479.10	Joback Method
dvisc	0.0001203	Pa×s	512.27	Joback Method
dvisc	0.0000734	Pa×s	545.45	Joback Method
dvisc	0.0000473	Pa×s	578.62	Joback Method
dvisc	0.0000320	Pa×s	611.79	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C607909&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
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