propyl 4-hydroxybenzoate

Other names: benzoic acid, 4-hydroxy-, propyl ester
propyl p-hydroxybenzoate
propylparaben
Inchi: InChI=1S/C10H12O3/c1-2-7-13-10(12)8-3-5-9(11)6-4-8/h3-6,11H,2,7H2,1H3
InchiKey: QELSKZZBTMNZEB-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: CCCOC(=O)c1ccc(O)cc1
Mol. weight [g/mol]: 180.20
CAS: 94-13-3

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
hsub	123.70 ± 0.60	kJ/mol	NIST Webbook
hvap	62.30	kJ/mol	Joback Method
log10ws	-2.59		Aqueous Solubility Prediction Method
logp	1.959		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
rinpol	1567.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	611.79	K	Joback Method
tc	835.24	K	Joback Method
tf	369.55	K	Ternary phase diagrams of ethyl paraben and propyl paraben in ethanol aqueous solvents
tf	369.40	K	Solubility and preferential solvation of some n-alkyl-parabens in methanol + water mixtures at 298.15 K
tf	369.20 ± 0.50	K	NIST Webbook
tf	369.90	K	Aqueous Solubility Prediction Method

vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.75	J/mol×K	798.00	Joback Method
cpg	394.42	J/mol×K	760.76	Joback Method
cpg	384.49	J/mol×K	723.51	Joback Method
cpg	373.90	J/mol×K	686.27	Joback Method
cpg	362.58	J/mol×K	649.03	Joback Method
cpg	350.48	J/mol×K	611.79	Joback Method
cpg	412.55	J/mol×K	835.24	Joback Method
dvisc	0.0008548	Pa×s	412.76	Joback Method
dvisc	0.0000320	Pa×s	611.79	Joback Method
dvisc	0.0000473	Pa×s	578.62	Joback Method
dvisc	0.0000734	Pa×s	545.45	Joback Method
dvisc	0.0001203	Pa×s	512.27	Joback Method
dvisc	0.0002113	Pa×s	479.10	Joback Method
dvisc	0.0004034	Pa×s	445.93	Joback Method
hfust	27.20	kJ/mol	369.30	NIST Webbook
hfust	27.99	kJ/mol	369.20	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94133&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Ternary phase diagrams of ethyl paraben and propyl paraben in ethanol + aqueous solvents: https://www.doi.org/10.1016/j.fluid.2014.05.036

Solubility and preferential solvation of some n-alkyl-parabens in methanol + water mixtures at 298.15 K: https://www.doi.org/10.1016/j.jct.2017.01.005

Solubility of Propylparahydroxybenzoate in Supercritical Carbon Dioxide with and Without Cosolvent: https://www.doi.org/10.1021/je049752p

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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