Propyl gallate

Other names:	3,4,5-Trihydroxybenzene-1-propylcarboxylate
	3,4,5-Trihydroxybenzoic acid n-propyl ester
	3,4,5-Trihydroxybenzoic acid, propyl ester
	Benzoic acid, 3,4,5-trihydroxy-, propyl ester
	Gallic acid n-propyl ester
	Gallic acid, propyl ester
	NCI-C505888
	NSC 2626
	Nipa 49
	Nipagallin P
	PG
	Progallin P
	Propyl 3,4,5-trihydroxybenzoate
	Propylester kyseliny gallove
	Tenox PG
	n-Propyl 3,4,5-trihydroxybenzoate
	n-Propyl ester of 3,4,5-trihydroxybenzoic acid
	n-Propyl gallate
Inchi:	InChI=1S/C10H12O5/c1-2-3-15-10(14)6-4-7(11)9(13)8(12)5-6/h4-5,11-13H,2-3H2,1H3
InchiKey:	ZTHYODDOHIVTJV-UHFFFAOYSA-N
Formula:	C10H12O5
SMILES:	CCCOC(=O)c1cc(O)c(O)c(O)c1
Mol. weight [g/mol]:	212.20
CAS:	121-79-9

Physical Properties

Property code	Value	Unit	Source
gf	-552.05	kJ/mol	Joback Method
hf	-789.93	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	88.33	kJ/mol	Joback Method
log10ws	-1.78		Aqueous Solubility Prediction Method
logp	1.370		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	5454.60	kPa	Joback Method
tb	773.03	K	Joback Method

tc	1012.07	K	Joback Method
tf	636.20	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.32	J/mol×K	773.03	Joback Method
cpg	484.09	J/mol×K	972.23	Joback Method
cpg	473.93	J/mol×K	932.39	Joback Method
cpg	464.15	J/mol×K	892.55	Joback Method
cpg	454.57	J/mol×K	852.71	Joback Method
cpg	445.02	J/mol×K	812.87	Joback Method
cpg	494.81	J/mol×K	1012.07	Joback Method
dvisc	6.7950144e-08	Pa×s	773.03	Joback Method
dvisc	9.7536895e-08	Pa×s	750.23	Joback Method
dvisc	0.0000001	Pa×s	727.42	Joback Method
dvisc	0.0000002	Pa×s	704.62	Joback Method
dvisc	0.0000003	Pa×s	681.81	Joback Method
dvisc	0.0000005	Pa×s	659.00	Joback Method
dvisc	0.0000009	Pa×s	636.20	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C121799&Units=SI

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

Solubilities of Gallic Acid and Its Esters in Water: https://www.doi.org/10.1021/je0601661

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume