

Ethyl gallate

Other names:	Ethyl 3,4,5-trihydroxybenzoate Benzoic acid, 3,4,5-trihydroxy-, ethyl ester Gallic acid ethyl ester Nipa No. 48 Nipagallin A Phyllembin Progallin A 3,4,5-Trihydroxybenzoic acid ethyl ester Ethylester kyseliny gallove NSC 402626
Inchi:	InChI=1S/C9H10O5/c1-2-14-9(13)5-3-6(10)8(12)7(11)4-5/h3-4,10-12H,2H2,1H3
InchiKey:	VFPFQHQNJCMNBZ-UHFFFAOYSA-N
Formula:	C9H10O5
SMILES:	CCOC(=O)c1cc(O)c(O)c(O)c1
Mol. weight [g/mol]:	198.17
CAS:	831-61-8

Physical Properties

Property code	Value	Unit	Source
gf	-560.47	kJ/mol	Joback Method
hf	-769.29	kJ/mol	Joback Method
hfus	33.24	kJ/mol	Joback Method
hvap	86.10	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.980		Crippen Method
mcvol	138.960	ml/mol	McGowan Method
pc	6318.86	kPa	Joback Method
tb	750.15	K	Joback Method
tc	993.90	K	Joback Method
tf	624.93	K	Joback Method
vc	0.353	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.85	J/mol×K	750.15	Joback Method
cpg	393.59	J/mol×K	790.77	Joback Method
cpg	402.16	J/mol×K	831.40	Joback Method
cpg	410.74	J/mol×K	872.02	Joback Method
cpg	419.52	J/mol×K	912.65	Joback Method
cpg	428.67	J/mol×K	953.27	Joback Method
cpg	438.38	J/mol×K	993.90	Joback Method
dvisc	0.0000011	Paxs	624.93	Joback Method
dvisc	0.0000007	Paxs	645.80	Joback Method
dvisc	0.0000004	Paxs	666.67	Joback Method
dvisc	0.0000003	Paxs	687.54	Joback Method
dvisc	0.0000002	Paxs	708.41	Joback Method
dvisc	0.0000001	Paxs	729.28	Joback Method
dvisc	9.8154782e-08	Paxs	750.15	Joback Method

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=C831618&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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