Tannic acid

Inchi: InChI=1S/C76H52O46/c77-32-1-22(2-33(78)53(32)92)67(103)113-47-16-27(11-42(87)58
InchiKey: LRBQNJMCXXYXIU-PPKXGCFTSA-N
Formula: C76H52O46
SMILES: O=C(OCC1OC(OC(=O)c2cc(O)c(O)c(OC(=O)c3cc(O)c(O)c(O)c3)c2)C(OC(=O)c2cc(O)c(
Mol. weight [g/mol]: 1701.20

Physical Properties

Property code	Value	Unit	Source
gf	-4632.22	kJ/mol	Joback Method
hf	-6343.81	kJ/mol	Joback Method
hfus	307.60	kJ/mol	Joback Method
hvap	631.45	kJ/mol	Joback Method
log10ws	-8.87		Crippen Method
logp	4.838		Crippen Method
mcvol	1060.260	ml/mol	McGowan Method
pc	9425.96	kPa	Joback Method
tb	5036.20	K	Joback Method
tf	4804.67	K	Joback Method
vc	2.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276145.14	J/mol×K	5036.20	Joback Method
cpg	83319.20	J/mol×K	3600.21	Joback Method
cpg	13586.18	J/mol×K	2164.23	Joback Method
cpg	2970.66	J/mol×K	728.24	Joback Method
dvisc	0.0000000	Pa×s	4804.67	Joback Method
dvisc	0.0000000	Pa×s	4843.26	Joback Method
dvisc	0.0000000	Pa×s	4881.85	Joback Method
dvisc	0.0000000	Pa×s	4920.43	Joback Method
dvisc	0.0000000	Pa×s	4959.02	Joback Method
dvisc	0.0000000	Pa×s	4997.61	Joback Method
dvisc	0.0000000	Pa×s	5036.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6006372&Units=SI

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
tf:	Normal melting (fusion) point
vc:	Critical Volume