Salicin

Other names:	2-(Hydroxymethyl)phenyl-«beta»-(d)-glucopyranoside, (d)-salicin
	2-(Hydroxymethyl)phenyl-«beta»-d-glucopyranoside
	2-(Hydroxymethyl)phenyl-Â«betaÂ»-(d)-glucopyranoside, (d)-salicin
	2-(Hydroxymethyl)phenyl-Â«betaÂ»-d-glucopyranoside
	Benzyl alcohol, o-hydroxy-, o-glucoside
	D-Salicin
	NSC 5751
	Salicine
	Salicoside
	Salicyl alcohol glucoside
	Saligenin-«beta»-D-glucopyranoside
	Saligenin-Â«betaÂ»-D-glucopyranoside
	o-(Hydroxymethyl)phenyl «beta»-D-glucopyranoside
	o-(Hydroxymethyl)phenyl Â«betaÂ»-D-glucopyranoside
	«alpha»-hydroxy-o-tolyl «beta»-D-glucopyranoside
	«beta»-D-Glucopyranoside, 2-(hydroxymethyl)phenyl
	Â«alphaÂ»-hydroxy-o-tolyl Â«betaÂ»-D-glucopyranoside
	Â«betaÂ»-D-Glucopyranoside, 2-(hydroxymethyl)phenyl
Inchi:	InChI=1S/C13H18O7/c14-5-7-3-1-2-4-8(7)19-13-12(18)11(17)10(16)9(6-15)20-13/h1-4,9
InchiKey:	NGFMICBWJRZIBI-UHFFFAOYSA-N
Formula:	C13H18O7
SMILES:	OCc1ccccc1OC1OC(CO)C(O)C(O)C1O
Mol. weight [g/mol]:	286.28
CAS:	138-52-3

Physical Properties

Property code	Value	Unit	Source
gf	-720.25	kJ/mol	Joback Method
hf	-1139.00	kJ/mol	Joback Method
hfus	48.80	kJ/mol	Joback Method
hvap	136.98	kJ/mol	Joback Method
log10ws	-0.85		Estimated Solubility Method
log10ws	-0.85		Aqueous Solubility Prediction Method
logp	-1.642		Crippen Method
mcvol	200.500	ml/mol	McGowan Method

pc	3704.46	kPa	Joback Method
rinpol	2572.00		NIST Webbook
tb	1039.64	K	Joback Method
tc	1281.59	K	Joback Method
tf	618.53	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.99	J/mol×K	1039.64	Joback Method
cpg	727.14	J/mol×K	1079.96	Joback Method
cpg	732.83	J/mol×K	1120.29	Joback Method
cpg	737.07	J/mol×K	1160.61	Joback Method
cpg	739.87	J/mol×K	1200.94	Joback Method
cpg	741.25	J/mol×K	1241.26	Joback Method
cpg	741.21	J/mol×K	1281.59	Joback Method
dvisc	0.0000077	Pa×s	618.53	Joback Method
dvisc	0.0000016	Pa×s	688.71	Joback Method
dvisc	0.0000004	Pa×s	758.90	Joback Method
dvisc	0.0000001	Pa×s	829.08	Joback Method
dvisc	6.0300289e-08	Pa×s	899.27	Joback Method
dvisc	2.7846737e-08	Pa×s	969.45	Joback Method
dvisc	1.4273610e-08	Pa×s	1039.64	Joback Method

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C138523&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume