Shikimic acid

Other names:	(-)-3,4,5-trihydroxy-1-cyclohexene-1-carboxylic acid
	(-)-shikimic acid
	(3R,4S,5R)-3,4,5-trihydroxy-1-cyclohexene-1-carboxylic acid
	(3R,4S,5R)-3,4,5-trihydroxycyclohex-1-enecarboxylic acid
	1-Cyclohexene-1-carboxylic acid, 3,4,5-trihydroxy-
	1-Cyclohexene-1-carboxylic acid, 3,4,5-trihydroxy-, [3R-(3«alpha»,4«alpha»,5«beta»)]-
	3,4,5-Trihydroxy-1-cyclohexene-1-carboxylic acid
	Bracken fern toxic component
	L-shikimic acid
	Shikimate
	Skikimic acid
Inchi:	InChI=1S/C7H10O5/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1,4-6,8-10H,2H2,(H,11,12)
InchiKey:	JXOHGGNKMLTUBP-UHFFFAOYSA-N
Formula:	C7H10O5
SMILES:	O=C(O)C1=CC(O)C(O)C(O)C1
Mol. weight [g/mol]:	174.15
CAS:	138-59-0

Physical Properties

Property code	Value	Unit	Source
gf	-638.78	kJ/mol	Joback Method
hf	-849.36	kJ/mol	Joback Method
hfus	26.65	kJ/mol	Joback Method
hvap	105.40	kJ/mol	Joback Method
log10ws	0.27		Crippen Method
logp	-1.516		Crippen Method
mcvol	119.380	ml/mol	McGowan Method
pc	5926.27	kPa	Joback Method
rinpol	2036.60		NIST Webbook
rinpol	2036.60		NIST Webbook
tb	796.50	K	Joback Method
tc	982.65	K	Joback Method
tf	460.15	K	Thermodynamic models for determination of the solubility of (-)-shikimic acid in different pure solvents and in (H2O + ethanol) binary solvent mixtures

vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.47	J/mol×K	796.50	Joback Method
cpg	401.16	J/mol×K	951.62	Joback Method
cpg	396.01	J/mol×K	920.60	Joback Method
cpg	390.38	J/mol×K	889.57	Joback Method
cpg	384.24	J/mol×K	858.55	Joback Method
cpg	377.61	J/mol×K	827.52	Joback Method
cpg	405.82	J/mol×K	982.65	Joback Method
dvisc	0.0000009	Pa×s	796.50	Joback Method
dvisc	0.0000018	Pa×s	742.76	Joback Method
dvisc	0.0000039	Pa×s	689.01	Joback Method
dvisc	0.0000098	Pa×s	635.27	Joback Method
dvisc	0.0000296	Pa×s	581.53	Joback Method
dvisc	0.0001116	Pa×s	527.78	Joback Method
dvisc	0.0005680	Pa×s	474.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C138590&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic models for determination of the solubility of (-)-shikimic acid in different pure solvents and in (H2O + ethanol) binary solvent mixtures:	https://www.doi.org/10.1016/j.jct.2015.04.009
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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