Sorbic Acid

Other names:	(2-Butenylidene)acetic acid
	(E,E)-2,4-hexadienoic acid
	(E,E)-Sorbic acid
	1,3-Pentadiene-1-carboxylic acid, (E,E)-
	2,4-Hexadienoic acid, (2E,4E)-
	2,4-Hexadienoic acid, (E,E)-
	2,4-Hexadienoic acid, (trans,trans)-
	2,4-hexadienoic acid
	2-Propenylacrylic acid
	2E,4E-Hexadienoic acid
	Acetic acid, (2-butenylidene)-
	Acetic acid, crotylidene-
	Crotylidene acetic acid
	E 200
	Hexa-2,4-dienoic acid, (E,E)-
	Hexadienoic acid, (E,E)
	Kyselina 1,3-pentadien-1-karboxylova
	Kyselina sorbova
	Panosorb
	Preservastat
	Sorbic acid, (E,E)-
	Sorbistat
	hexa-2,4-dienoic acid
	trans,trans-2,4-Hexadienoic acid
	trans,trans-Sorbic acid
	«alpha»-trans-«gamma»-trans-Sorbic acid
	Â«alphaÂ»-trans-Â«gammaÂ»-trans-Sorbic acid
Inchi:	InChI=1S/C6H8O2/c1-2-3-4-5-6(7)8/h2-5H,1H3,(H,7,8)/b3-2+,5-4+
InchiKey:	WSWCOQWTEOXDQX-MQQKCMAXSA-N
Formula:	C6H8O2
SMILES:	CC=CC=CC(=O)O
Mol. weight [g/mol]:	112.13
CAS:	110-44-1

Physical Properties

Property code	Value	Unit	Source

chl	-3125.80	kJ/mol	NIST Webbook
chs	-3123.00	kJ/mol	NIST Webbook
gf	-105.66	kJ/mol	Joback Method
hf	-197.54	kJ/mol	Joback Method
hfus	17.39	kJ/mol	Joback Method
hvap	52.29	kJ/mol	Joback Method
log10ws	-1.77		Aqueous Solubility Prediction Method
logp	1.203		Crippen Method
mcvol	94.240	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
rinpol	1056.00		NIST Webbook
ripol	2150.00		NIST Webbook
ripol	2150.00		NIST Webbook
tb	491.05	K	Joback Method
tc	678.28	K	Joback Method
tf	407.65	K	NIST Webbook
tf	407.32	K	Aqueous Solubility Prediction Method
tf	405.30	K	Solubility and solution thermodynamics of sorbic acid in eight pure organic solvents
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.33	J/mol×K	491.05	Joback Method
cpg	196.17	J/mol×K	522.25	Joback Method
cpg	203.56	J/mol×K	553.46	Joback Method
cpg	210.51	J/mol×K	584.66	Joback Method
cpg	217.05	J/mol×K	615.87	Joback Method
cpg	223.22	J/mol×K	647.07	Joback Method
cpg	229.03	J/mol×K	678.28	Joback Method
dvisc	0.0235893	Pa×s	257.97	Joback Method
dvisc	0.0057171	Pa×s	296.82	Joback Method
dvisc	0.0019236	Pa×s	335.66	Joback Method
dvisc	0.0008113	Pa×s	374.51	Joback Method
dvisc	0.0004025	Pa×s	413.36	Joback Method
dvisc	0.0002252	Pa×s	452.20	Joback Method
dvisc	0.0001381	Pa×s	491.05	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility and solution thermodynamics of sorbic acid in eight pure organic solvents:	https://www.doi.org/10.1016/j.jct.2015.02.004

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume