

RESVERATROL

Other names:	1,3-Benzenediol, 5-[(1E)-2-(4-hydroxyphenyl)ethenyl]- 1,3-Benzenediol, 5-[2-(4-hydroxyphenyl)ethenyl]-, (E)- 5-[(1E)-2-(4-hydroxyphenyl)-ethenyl]-1,3-benzenediol trans-resveratrol
Inchi:	InChI=1S/C14H12O3/c15-12-5-3-10(4-6-12)1-2-11-7-13(16)9-14(17)8-11/h1-9,15-17H/b2
InchiKey:	LUKBXSAWLPMMSZ-OWOJBTEDSA-N
Formula:	C14H12O3
SMILES:	Oc1ccc(C=Cc2cc(O)cc(O)c2)cc1
Mol. weight [g/mol]:	228.24
CAS:	501-36-0

Physical Properties

Property code	Value	Unit	Source
gf	-91.82	kJ/mol	Joback Method
hf	-273.94	kJ/mol	Joback Method
hfus	37.65	kJ/mol	Joback Method
hvap	90.31	kJ/mol	Joback Method
log10ws	-4.34		Aqueous Solubility Prediction Method
logp	2.974		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	5094.76	kPa	Joback Method
tb	819.10	K	Joback Method
tc	1090.14	K	Joback Method
tf	541.30	K	Measurement and correlation of solubility of trans-resveratrol in 11 solvents at T = (278.2, 288.2, 298.2, 308.2, and 318.2) K
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.77	J/mol×K	819.10	Joback Method

cpg	502.76	J/mol×K	864.27	Joback Method
cpg	514.92	J/mol×K	909.45	Joback Method
cpg	527.60	J/mol×K	954.62	Joback Method
cpg	541.16	J/mol×K	999.79	Joback Method
cpg	555.98	J/mol×K	1044.97	Joback Method
cpg	572.40	J/mol×K	1090.14	Joback Method
dvisc	0.0000009	Pa×s	630.46	Joback Method
dvisc	0.0000004	Pa×s	661.90	Joback Method
dvisc	0.0000002	Pa×s	693.34	Joback Method
dvisc	0.0000001	Pa×s	724.78	Joback Method
dvisc	7.7542175e-08	Pa×s	756.22	Joback Method
dvisc	4.7688180e-08	Pa×s	787.66	Joback Method
dvisc	3.0443261e-08	Pa×s	819.10	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/AqueousDataset002.xlsx>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C501360&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Measurement and correlation of solubility of trans-resveratrol in 11 solvents at (278.2, 298.2, 308.2, 318.2, 328.2, 338.2, 348.2, 358.2, 368.2, 378.2, 388.2) K
Measurement and correlation of solubility of trans-resveratrol in Ethanol + Water and Acetone + Water Mixed Solvents at Different Temperatures:

<https://www.doi.org/10.1016/j.jct.2007.10.006>

<https://www.doi.org/10.1021/je800410b>

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
tc:	Critical Temperature

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

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