

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

Sources

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/ci9903071
Measurement and correlation of solubility of trans-resveratrol in 11 Measurement (278.0 to 298.2, Solubilities 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 https://en.wikipedia.org/wiki/Joback_method

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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