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=C/c2cc(O)cc(O)c2)cc1
Mol. weight [g/mol]: 228.25

Physical Properties

Property code	Value	Unit	Source
hf	-262.78	kJ/mol	Cheméo Relay (1.0)
hfus	37.65	kJ/mol	Joback Method
hvap	149.58	kJ/mol	Cheméo Relay (1.0)
ie	7.51	eV	Cheméo Relay (1.0)
log10ws	-4.34		Aqueous Solubility Prediction Method
logp	2.974		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
tb	667.55	K	Cheméo Relay (1.0)
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

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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:	https://www.doi.org/10.1016/j.jct.2007.10.006
Measurement and Correlation of Solubilities of trans-Resveratrol in Ethanol + Water and Acetone + Water Mixed Solvents at Different Temperatures:	https://www.doi.org/10.1021/je800410b
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C501360&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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