PHENOL, 4-(2-PHENYLETHENYL)-

Other names: Hydroxystlbene,4-
4-Hydroxyphenylstilbene
4-Hydroxystilbene
4-Stilbenol
4-[2-Phenylethenyl]phenol
stilben-4-ol

Inchi: InChI=1S/C14H12O/c15-14-10-8-13(9-11-14)7-6-12-4-2-1-3-5-12/h1-11,15H/b7-6-

InchiKey: QVLMUEOXQBUPAH-VOTSOKGWSA-N

Formula: C14H12O

SMILES: Oc1ccc(/C=C/c2ccccc2)cc1

Mol. weight [g/mol]: 196.25

Physical Properties

Property code	Value	Unit	Source
af	0.5734		Cheméo Relay (1.0)
gf	217.42	kJ/mol	Joback Method
hf	67.75	kJ/mol	Cheméo Relay (1.0)
hfus	26.08	kJ/mol	Joback Method
hvap	98.36	kJ/mol	Cheméo Relay (1.0)
ie	7.54	eV	Cheméo Relay (1.0)
log10ws	-3.59		Cheméo Relay (1.0)
logp	3.563		Crippen Method
mcvol	162.170	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	281.30		NIST Webbook
rinpol	281.30		NIST Webbook
tb	628.20	K	Cheméo Relay (1.0)
tc	888.62	K	Cheméo Relay (1.0)
tf	462.92	K	Cheméo Relay (1.0)
vc	0.567	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	404.38	J/mol×K	657.86	Joback Method
cpg	418.97	J/mol×K	701.15	Joback Method
cpg	432.33	J/mol×K	744.43	Joback Method
cpg	444.66	J/mol×K	787.72	Joback Method
cpg	456.14	J/mol×K	831.01	Joback Method
cpg	466.96	J/mol×K	874.29	Joback Method
cpg	477.31	J/mol×K	917.58	Joback Method
dvisc	0.0008923	Pa×s	407.02	Joback Method
dvisc	0.0003425	Pa×s	448.83	Joback Method
dvisc	0.0001547	Pa×s	490.63	Joback Method
dvisc	0.0000792	Pa×s	532.44	Joback Method
dvisc	0.0000447	Pa×s	574.25	Joback Method
dvisc	0.0000273	Pa×s	616.05	Joback Method
dvisc	0.0000177	Pa×s	657.86	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3839461&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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
ie: Ionization energy
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