Ethanedione,(4-hydroxyphenyl)phenyl-

Other names:	1-(4-Hydroxyphenyl)-2-phenylethan-1,2-dion
	1-(4-Hydroxyphenyl)-2-phenylethane-1,2-dione
Inchi:	InChI=1S/C14H10O3/c15-12-8-6-11(7-9-12)14(17)13(16)10-4-2-1-3-5-10/h1-9,15H
InchiKey:	IVUXDMQTCNWTDP-UHFFFAOYSA-N
Formula:	C14H10O3
SMILES:	O=C(C(=O)c1ccc(O)cc1)c1ccccc1
Mol. weight [g/mol]:	226.23
CAS:	38469-73-7

Physical Properties

Property code	Value	Unit	Source
gf	-120.64	kJ/mol	Joback Method
hf	-261.70	kJ/mol	Joback Method
hfus	29.08	kJ/mol	Joback Method
hvap	77.82	kJ/mol	Joback Method
ie	8.90 ± 0.05	eV	NIST Webbook
log10ws	-3.15		Crippen Method
logp	2.458		Crippen Method
mcvol	169.610	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	761.44	K	Joback Method
tc	1020.48	K	Joback Method
tf	511.96	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.68	J/mol×K	761.44	Joback Method
cpg	461.33	J/mol×K	804.61	Joback Method
cpg	472.08	J/mol×K	847.79	Joback Method
cpg	482.07	J/mol×K	890.96	Joback Method
cpg	491.47	J/mol×K	934.14	Joback Method
cpg	500.43	J/mol×K	977.31	Joback Method

cpg	509.10	J/mol×K	1020.48	Joback Method
dvisc	0.0002761	Pa×s	511.96	Joback Method
dvisc	0.0001385	Pa×s	553.54	Joback Method
dvisc	0.0000765	Pa×s	595.12	Joback Method
dvisc	0.0000457	Pa×s	636.70	Joback Method
dvisc	0.0000291	Pa×s	678.28	Joback Method
dvisc	0.0000195	Pa×s	719.86	Joback Method
dvisc	0.0000136	Pa×s	761.44	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38469737&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie: Ionization energy
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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