(2E)-1,3-bis(4-hydroxyphenyl)-2-buten-1-one

Inchi: InChI=1S/C16H14O3/c1-11(12-2-6-14(17)7-3-12)10-16(19)13-4-8-15(18)9-5-13/h2-10,17
InchiKey: HBEIHQWBXCHEKJ-ZHACJKMWSA-N
Formula: C16H14O3
SMILES: CC(=CC(=O)c1ccc(O)cc1)c1ccc(O)cc1
Mol. weight [g/mol]: 254.28
CAS: 57558-57-3

Physical Properties

Property code	Value	Unit	Source
gf	-57.83	kJ/mol	Joback Method
hf	-260.28	kJ/mol	Joback Method
hfus	37.34	kJ/mol	Joback Method
hvap	88.57	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.384		Crippen Method
mcvol	197.790	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	837.99	K	Joback Method
tc	1100.33	K	Joback Method
tf	577.25	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.25	J/mol×K	837.99	Joback Method
cpg	576.22	J/mol×K	881.71	Joback Method
cpg	588.93	J/mol×K	925.44	Joback Method
cpg	601.63	J/mol×K	969.16	Joback Method
cpg	614.61	J/mol×K	1012.88	Joback Method
cpg	628.12	J/mol×K	1056.61	Joback Method
cpg	642.45	J/mol×K	1100.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57558573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

cpg:	Ideal gas heat capacity
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