ETHANONE, 2-HYDROXY-1,2-BIS(4-METHOXYPHENYL)-

Other names: p-Anisoin
Benzoin, 4,4'-dimethoxy-
4,4'-Dimethoxybenzoin
p,p'-Dimethoxybenzoin
Anisoin
4,4'-anisoin

Inchi: InChI=1S/C16H16O4/c1-19-13-7-3-11(4-8-13)15(17)16(18)12-5-9-14(20-2)10-6-12/h3-10

InchiKey: LRRQSCPPOIUNGX-UHFFFAOYSA-N

Formula: C16H16O4

SMILES: COc1ccc(C(=O)C(O)c2ccc(OC)cc2)cc1

Mol. weight [g/mol]: 272.30

Physical Properties

Property code	Value	Unit	Source
hf	-451.82	kJ/mol	Cheméo Relay (1.0)
hfus	29.04	kJ/mol	Joback Method
hvap	109.68	kJ/mol	Cheméo Relay (1.0)
ie	7.96	eV	Cheméo Relay (1.0)
log10ws	-2.97		Cheméo Relay (1.0)
logp	2.620		Crippen Method
mcvol	207.960	ml/mol	McGowan Method
tb	636.09	K	Cheméo Relay (1.0)
tf	383.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.90	J/mol×K	819.25	Joback Method
cpg	609.05	J/mol×K	855.96	Joback Method
cpg	620.16	J/mol×K	892.67	Joback Method
cpg	630.25	J/mol×K	929.38	Joback Method
cpg	639.35	J/mol×K	966.09	Joback Method
cpg	647.47	J/mol×K	1002.80	Joback Method
cpg	654.63	J/mol×K	1039.51	Joback Method

dvisc	0.0004352	Pa×s	488.17	Joback Method
dvisc	0.0001882	Pa×s	543.35	Joback Method
dvisc	0.0000950	Pa×s	598.53	Joback Method
dvisc	0.0000538	Pa×s	653.71	Joback Method
dvisc	0.0000333	Pa×s	708.89	Joback Method
dvisc	0.0000221	Pa×s	764.07	Joback Method
dvisc	0.0000155	Pa×s	819.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119528&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):	
Cheméo Relay (1.0, beta):	

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