4,4'-Dimethoxybenzhydrol

Other names: Benzenemethanol, 4-methoxy-«alpha»-(4-methoxyphenyl)-
p,p'-Dimethoxybenzhydrol
Benzhydrol, 4,4'-dimethoxy-
Bis(p-methoxyphenyl)carbinol
4-Methoxy-4'-methoxybenzhydrol
p,p'-dimethoxybenzhydryl alcohol

Inchi: InChI=1S/C15H16O3/c1-17-13-7-3-11(4-8-13)15(16)12-5-9-14(18-2)10-6-12/h3-10,15-16

InchiKey: ZODAOVNETBTTJX-UHFFFAOYSA-N

Formula: C15H16O3

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

Mol. weight [g/mol]: 244.29

CAS: 728-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-68.28	kJ/mol	Joback Method
hf	-324.76	kJ/mol	Joback Method
hfus	24.85	kJ/mol	Joback Method
hvap	75.97	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.785		Crippen Method
mcvol	192.300	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
tb	742.50	K	Joback Method
tc	959.56	K	Joback Method
tf	426.97	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.37	J/mol×K	742.50	Joback Method
cpg	543.92	J/mol×K	778.68	Joback Method
cpg	556.49	J/mol×K	814.85	Joback Method

cpg	568.10	J/mol×K	851.03	Joback Method
cpg	578.78	J/mol×K	887.21	Joback Method
cpg	588.54	J/mol×K	923.38	Joback Method
cpg	597.40	J/mol×K	959.56	Joback Method
dvisc	0.0008150	Pa×s	426.97	Joback Method
dvisc	0.0003160	Pa×s	479.56	Joback Method
dvisc	0.0001478	Pa×s	532.15	Joback Method
dvisc	0.0000792	Pa×s	584.74	Joback Method
dvisc	0.0000471	Pa×s	637.32	Joback Method
dvisc	0.0000303	Pa×s	689.91	Joback Method
dvisc	0.0000207	Pa×s	742.50	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=C728870&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
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