

Acetophenone, 2',4'-dihydroxy-2-(p-methoxyphenyl)-

Inchi:	InChI=1S/C15H14O4/c1-19-12-5-2-10(3-6-12)8-14(17)13-7-4-11(16)9-15(13)18/h2-7,9,1
InchiKey:	XHBZOAYMBBUURD-UHFFFAOYSA-N
Formula:	C15H14O4
SMILES:	COc1ccc(CC(=O)c2ccc(O)cc2O)cc1
Mol. weight [g/mol]:	258.27
CAS:	487-49-0

Physical Properties

Property code	Value	Unit	Source
gf	-252.55	kJ/mol	Joback Method
hf	-490.76	kJ/mol	Joback Method
hfus	36.65	kJ/mol	Joback Method
hvap	89.38	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.532		Crippen Method
mcvol	193.870	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
tb	838.47	K	Joback Method
tc	1089.81	K	Joback Method
tf	619.77	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.70	J/molxK	838.47	Joback Method
cpg	572.04	J/molxK	880.36	Joback Method
cpg	583.95	J/molxK	922.25	Joback Method
cpg	595.58	J/molxK	964.14	Joback Method
cpg	607.12	J/molxK	1006.03	Joback Method
cpg	618.75	J/molxK	1047.92	Joback Method
cpg	630.64	J/molxK	1089.81	Joback Method
dvisc	0.0000077	Paxs	619.77	Joback Method
dvisc	0.0000041	Paxs	656.22	Joback Method

dvisc	0.0000023	Paxs	692.67	Joback Method
dvisc	0.0000014	Paxs	729.12	Joback Method
dvisc	0.0000009	Paxs	765.57	Joback Method
dvisc	0.0000006	Paxs	802.02	Joback Method
dvisc	0.0000004	Paxs	838.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C487490&Units=SI

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

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