5-Hydroxy-4-methoxy-6-phenethyl-5,6-dihydro-2H

Inchi: InChI=1S/C14H16O4/c1-17-12-9-13(15)18-11(14(12)16)8-7-10-5-3-2-4-6-10/h2-6,9,11,14
InchiKey: VJCNEDVMYQCMBK-UHFFFAOYSA-N
Formula: C14H16O4
SMILES: COC1=CC(=O)OC(CCc2ccccc2)C1O
Mol. weight [g/mol]: 248.27
CAS: 78376-49-5

Physical Properties

Property code	Value	Unit	Source
gf	-234.05	kJ/mol	Joback Method
hf	-569.62	kJ/mol	Joback Method
hfus	32.56	kJ/mol	Joback Method
hvap	77.95	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.436		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
rinpol	2320.60		NIST Webbook
rinpol	2320.60		NIST Webbook
tb	774.79	K	Joback Method
tc	997.05	K	Joback Method
tf	468.22	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.16	J/mol×K	774.79	Joback Method
cpg	581.60	J/mol×K	811.83	Joback Method
cpg	594.85	J/mol×K	848.88	Joback Method
cpg	606.89	J/mol×K	885.92	Joback Method
cpg	617.71	J/mol×K	922.96	Joback Method
cpg	627.31	J/mol×K	960.00	Joback Method
cpg	635.68	J/mol×K	997.05	Joback Method

Sources

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=C78376495&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume