4-Methoxy-6-(4-methoxyphenethyl)-5,6-dihydro-2H

Inchi: InChI=1S/C15H18O4/c1-17-12-6-3-11(4-7-12)5-8-13-9-14(18-2)10-15(16)19-13/h3-4,6-7
InchiKey: IZGFAKZIDOQLHS-UHFFFAOYSA-N
Formula: C15H18O4
SMILES: COC1=CC(=O)OC(CCc2ccc(OC)cc2)C1
Mol. weight [g/mol]: 262.30
CAS: 3328-59-4

Physical Properties

Property code	Value	Unit	Source
gf	-195.73	kJ/mol	Joback Method
hf	-561.38	kJ/mol	Joback Method
hfus	30.79	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.474		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tb	737.56	K	Joback Method
tc	970.63	K	Joback Method
tf	457.66	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.99	J/mol×K	737.56	Joback Method
cpg	604.50	J/mol×K	776.41	Joback Method
cpg	620.65	J/mol×K	815.25	Joback Method
cpg	635.41	J/mol×K	854.10	Joback Method
cpg	648.76	J/mol×K	892.94	Joback Method
cpg	660.67	J/mol×K	931.79	Joback Method
cpg	671.11	J/mol×K	970.63	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=C3328594&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