4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dimethoxy-2-phenyl-

Other names: Flavanone, 5,7-dimethoxy-
5,7-Dimethoxyflavanone
5,7-Dimethoxy-2-phenylchroman-4-one

Inchi: InChI=1S/C17H16O4/c1-19-12-8-15(20-2)17-13(18)10-14(21-16(17)9-12)11-6-4-3-5-7-11

InchiKey: IAFBOKYTDSDNHV-UHFFFAOYSA-N

Formula: C17H16O4

SMILES: COc1cc(OC)c2c(c1)OC(c1ccccc1)CC2=O

Mol. weight [g/mol]: 284.31

CAS: 1036-72-2

Physical Properties

Property code	Value	Unit	Source
gf	-81.87	kJ/mol	Joback Method
hf	-423.06	kJ/mol	Joback Method
hfus	32.60	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.410		Crippen Method
mcvol	211.190	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	2570.90		NIST Webbook
rinpol	2570.90		NIST Webbook
tb	807.28	K	Joback Method
tc	1057.67	K	Joback Method
tf	525.42	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.62	J/mol×K	807.28	Joback Method
cpg	642.56	J/mol×K	849.01	Joback Method
cpg	656.96	J/mol×K	890.74	Joback Method
cpg	669.81	J/mol×K	932.48	Joback Method

cpg	681.14	J/mol×K	974.21	Joback Method
cpg	690.93	J/mol×K	1015.94	Joback Method
cpg	699.19	J/mol×K	1057.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1036722&Units=SI

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