5,7-Dimethoxy-2-(4-methoxyphenyl)chroman-4-on

Inchi: InChI=1S/C18H18O5/c1-20-12-6-4-11(5-7-12)15-10-14(19)18-16(22-3)8-13(21-2)9-17(18

InchiKey: MQFSCAHSIUPLSB-UHFFFAOYSA-N

Formula: C18H18O5

SMILES: COc1ccc(C2CC(=O)c3c(OC)cc(OC)cc3O2)cc1

Mol. weight [g/mol]: 314.33

CAS: 66074-95-1

Physical Properties

Property code	Value	Unit	Source
gf	-188.08	kJ/mol	Joback Method
hf	-587.39	kJ/mol	Joback Method
hfus	35.99	kJ/mol	Joback Method
hvap	78.93	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.419		Crippen Method
mcvol	231.150	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	2855.40		NIST Webbook
rinpol	2855.40		NIST Webbook
tb	857.56	K	Joback Method
tc	1100.83	K	Joback Method
tf	571.44	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.95	J/mol×K	857.56	Joback Method
cpg	723.98	J/mol×K	898.10	Joback Method
cpg	737.36	J/mol×K	938.65	Joback Method
cpg	749.07	J/mol×K	979.19	Joback Method
cpg	759.08	J/mol×K	1019.74	Joback Method
cpg	767.38	J/mol×K	1060.28	Joback Method
cpg	773.93	J/mol×K	1100.83	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=C66074951&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