3-(2,4-dimethoxyphenyl)chroman-7-ol

Inchi: InChI=1S/C17H18O4/c1-19-14-5-6-15(17(9-14)20-2)12-7-11-3-4-13(18)8-16(11)21-10-12
InchiKey: TUXCLJQCYVCGDW-UHFFFAOYSA-N
Formula: C17H18O4
SMILES: COc1ccc(C2COc3cc(O)ccc3C2)c(OC)c1
Mol. weight [g/mol]: 286.32
CAS: 71831-00-0

Physical Properties

Property code	Value	Unit	Source
gf	-113.90	kJ/mol	Joback Method
hf	-462.67	kJ/mol	Joback Method
hfus	38.87	kJ/mol	Joback Method
hvap	82.40	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.128		Crippen Method
mcvol	215.490	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	2687.90		NIST Webbook
rinpol	2687.90		NIST Webbook
tb	820.08	K	Joback Method
tc	1067.06	K	Joback Method
tf	568.92	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.35	J/mol×K	820.08	Joback Method
cpg	665.76	J/mol×K	861.24	Joback Method
cpg	680.13	J/mol×K	902.41	Joback Method
cpg	693.57	J/mol×K	943.57	Joback Method
cpg	706.17	J/mol×K	984.74	Joback Method
cpg	718.06	J/mol×K	1025.90	Joback Method
cpg	729.33	J/mol×K	1067.06	Joback Method

dvisc	0.0001023	Pa×s	568.92	Joback Method
dvisc	0.0000595	Pa×s	610.78	Joback Method
dvisc	0.0000370	Pa×s	652.64	Joback Method
dvisc	0.0000244	Pa×s	694.50	Joback Method
dvisc	0.0000169	Pa×s	736.36	Joback Method
dvisc	0.0000122	Pa×s	778.22	Joback Method
dvisc	0.0000090	Pa×s	820.08	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=C71831000&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume