(1S,2R)-2-(4-allyl-2,6-Dimethoxyphenoxy)-1-(3,4,5-

Inchi: InChI=1S/C23H30O7/c1-8-9-15-10-17(25-3)23(18(11-15)26-4)30-14(2)21(24)16-12-19(2

InchiKey: KKEKLEUWEJUCRA-UHFFFAOYSA-N

Formula: C23H30O7

SMILES: C=CCc1cc(OC)c(OC(C)C(O)c2cc(OC)c(OC)c(OC)c2)c(OC)c1

Mol. weight [g/mol]: 418.48

CAS: 52190-20-2

Physical Properties

Property code	Value	Unit	Source
gf	-374.04	kJ/mol	Joback Method
hf	-944.49	kJ/mol	Joback Method
hfus	43.96	kJ/mol	Joback Method
hvap	105.01	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	3.959		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
pc	1270.06	kPa	Joback Method
rinpol	2970.90		NIST Webbook
rinpol	2970.90		NIST Webbook
tb	1031.38	K	Joback Method
tc	1262.70	K	Joback Method
tf	639.37	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.92	J/mol×K	1031.38	Joback Method
cpg	1093.11	J/mol×K	1224.15	Joback Method
cpg	1091.58	J/mol×K	1185.59	Joback Method
cpg	1087.75	J/mol×K	1147.04	Joback Method
cpg	1081.66	J/mol×K	1108.49	Joback Method
cpg	1073.37	J/mol×K	1069.93	Joback Method
cpg	1092.29	J/mol×K	1262.70	Joback Method

dvisc	0.0000015	Pa×s	1031.38	Joback Method
dvisc	0.0000020	Pa×s	966.05	Joback Method
dvisc	0.0000029	Pa×s	900.71	Joback Method
dvisc	0.0000043	Pa×s	835.38	Joback Method
dvisc	0.0000070	Pa×s	770.04	Joback Method
dvisc	0.0000123	Pa×s	704.71	Joback Method
dvisc	0.0000244	Pa×s	639.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52190202&Units=SI
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

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