(1S,2R)-2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4-d acetate

Inchi: InChI=1S/C24H30O7/c1-8-9-17-12-21(28-6)24(22(13-17)29-7)30-15(2)23(31-16(3)25)18
InchiKey: SITDJJDXDVFCAP-UHFFFAOYSA-N
Formula: C24H30O7
SMILES: C=CCc1cc(OC)c(OC(C)C(OC(C)=O)c2ccc(OC)c(OC)c2)c(OC)c1
Mol. weight [g/mol]: 430.49
CAS: 1257094-34-0

Physical Properties

Property code	Value	Unit	Source
gf	-348.09	kJ/mol	Joback Method
hf	-914.01	kJ/mol	Joback Method
hfus	44.45	kJ/mol	Joback Method
hvap	96.64	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.521		Crippen Method
mcvol	333.990	ml/mol	McGowan Method
pc	1176.05	kPa	Joback Method
rinpol	2853.90		NIST Webbook
rinpol	2853.90		NIST Webbook
tb	1010.97	K	Joback Method
tc	1240.40	K	Joback Method
tf	627.23	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1081.53	J/mol×K	1010.97	Joback Method
cpg	1093.04	J/mol×K	1049.21	Joback Method
cpg	1102.41	J/mol×K	1087.45	Joback Method
cpg	1109.59	J/mol×K	1125.69	Joback Method
cpg	1114.55	J/mol×K	1163.92	Joback Method
cpg	1117.24	J/mol×K	1202.16	Joback Method
cpg	1117.63	J/mol×K	1240.40	Joback Method

dvisc	0.0000767	Pa×s	627.23	Joback Method
dvisc	0.0000466	Pa×s	691.19	Joback Method
dvisc	0.0000309	Pa×s	755.14	Joback Method
dvisc	0.0000218	Pa×s	819.10	Joback Method
dvisc	0.0000162	Pa×s	883.06	Joback Method
dvisc	0.0000125	Pa×s	947.01	Joback Method
dvisc	0.0000100	Pa×s	1010.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1257094340&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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