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

Inchi: InChI=1S/C22H28O6/c1-7-8-15-11-19(26-5)22(20(12-15)27-6)28-14(2)21(23)16-9-10-17
InchiKey: IQBXVNSNERBTIG-UHFFFAOYSA-N
Formula: C22H28O6
SMILES: C=CCc1cc(OC)c(OC(C)C(O)c2ccc(OC)c(OC)c2)c(OC)c1
Mol. weight [g/mol]: 388.45
CAS: 162409-91-8

Physical Properties

Property code	Value	Unit	Source
gf	-267.83	kJ/mol	Joback Method
hf	-780.16	kJ/mol	Joback Method
hfus	40.57	kJ/mol	Joback Method
hvap	99.71	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	3.950		Crippen Method
mcvol	304.240	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	2870.30		NIST Webbook
rinpol	2870.30		NIST Webbook
tb	981.10	K	Joback Method
tc	1203.15	K	Joback Method
tf	593.35	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.42	J/mol×K	981.10	Joback Method
cpg	1022.70	J/mol×K	1166.14	Joback Method
cpg	1017.53	J/mol×K	1129.13	Joback Method
cpg	1010.60	J/mol×K	1092.12	Joback Method
cpg	1001.92	J/mol×K	1055.12	Joback Method
cpg	991.52	J/mol×K	1018.11	Joback Method
cpg	1026.08	J/mol×K	1203.15	Joback Method

dvisc	0.0000024	Pa×s	981.10	Joback Method
dvisc	0.0000033	Pa×s	916.48	Joback Method
dvisc	0.0000049	Pa×s	851.85	Joback Method
dvisc	0.0000075	Pa×s	787.23	Joback Method
dvisc	0.0000126	Pa×s	722.60	Joback Method
dvisc	0.0000234	Pa×s	657.98	Joback Method
dvisc	0.0000495	Pa×s	593.35	Joback Method

Sources

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=C162409918&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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