(S)-5-Allyl-2-((1-(3,4-dimethoxyphenyl)propan-2-yl

Inchi: InChI=1S/C22H28O5/c1-7-8-16-13-20(25-5)22(21(14-16)26-6)27-15(2)11-17-9-10-18(23

InchiKey: RZMDLBAIWHLFEF-OAHLLOKOSA-N

Formula: C22H28O5

SMILES: C=CCc1cc(OC)c(OC(C)Cc2ccc(OC)c(OC)c2)c(OC)c1

Mol. weight [g/mol]: 372.45

CAS: 1246343-70-3

Physical Properties

Property code	Value	Unit	Source
gf	-128.57	kJ/mol	Joback Method
hf	-622.65	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	83.42	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.459		Crippen Method
mcvol	298.370	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	2653.00		NIST Webbook
rinpol	2653.00		NIST Webbook
tb	889.36	K	Joback Method
tc	1104.75	K	Joback Method
tf	547.53	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.17	J/mol×K	889.36	Joback Method
cpg	938.86	J/mol×K	925.26	Joback Method
cpg	953.03	J/mol×K	961.16	Joback Method
cpg	965.64	J/mol×K	997.05	Joback Method
cpg	976.67	J/mol×K	1032.95	Joback Method
cpg	986.12	J/mol×K	1068.85	Joback Method
cpg	993.94	J/mol×K	1104.75	Joback Method

dvisc	0.0001426	Pa×s	547.53	Joback Method
dvisc	0.0000884	Pa×s	604.50	Joback Method
dvisc	0.0000595	Pa×s	661.47	Joback Method
dvisc	0.0000427	Pa×s	718.45	Joback Method
dvisc	0.0000321	Pa×s	775.42	Joback Method
dvisc	0.0000252	Pa×s	832.39	Joback Method
dvisc	0.0000203	Pa×s	889.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1246343703&Units=SI

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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