

(S)-5-Allyl-1,3-dimethoxy-2-((1-(3,4,5-trimethoxyph

Inchi:	InChI=1S/C23H30O6/c1-8-9-16-11-20(26-5)23(21(12-16)27-6)29-15(2)10-17-13-18(24-3
InchiKey:	ZOPUPXKPXCSWAE-OAHLLOKOSA-N
Formula:	C23H30O6
SMILES:	C=CCc1cc(OC)c(OC(C)Cc2cc(OC)c(OC)c(OC)c2)c(OC)c1
Mol. weight [g/mol]:	402.48
CAS:	836632-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-234.78	kJ/mol	Joback Method
hf	-786.98	kJ/mol	Joback Method
hfus	43.40	kJ/mol	Joback Method
hvap	88.72	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.468		Crippen Method
mvol	318.330	ml/mol	McGowan Method
pc	1184.16	kPa	Joback Method
rinpol	2766.30		NIST Webbook
rinpol	2766.30		NIST Webbook
tb	939.64	K	Joback Method
tc	1157.63	K	Joback Method
tf	593.55	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.52	J/molxK	939.64	Joback Method
cpg	1025.03	J/molxK	975.97	Joback Method
cpg	1037.76	J/molxK	1012.30	Joback Method
cpg	1048.64	J/molxK	1048.63	Joback Method
cpg	1057.64	J/molxK	1084.97	Joback Method
cpg	1064.72	J/molxK	1121.30	Joback Method
cpg	1069.83	J/molxK	1157.63	Joback Method

dvisc	0.0000841	Paxs	593.55	Joback Method
dvisc	0.0000542	Paxs	651.23	Joback Method
dvisc	0.0000375	Paxs	708.91	Joback Method
dvisc	0.0000275	Paxs	766.60	Joback Method
dvisc	0.0000210	Paxs	824.28	Joback Method
dvisc	0.0000166	Paxs	881.96	Joback Method
dvisc	0.0000136	Paxs	939.64	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C836632587&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
mvol:	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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