

(1S,2R)-2-(4-Allyl-2-methoxyphenoxy)-1-(3,4,5-trimethoxyphenyl)ethane

Inchi:	InChI=1S/C22H28O6/c1-7-8-15-9-10-17(18(11-15)24-3)28-14(2)21(23)16-12-19(25-4)22
InchiKey:	RKIYTFCMWRXPHL-UHFFFAOYSA-N
Formula:	C22H28O6
SMILES:	<chem>C=CCc1ccc(OC(C)C(O)c2cc(OC)c(OC)c(OC)c2)c(OC)c1</chem>
Mol. weight [g/mol]:	388.45
CAS:	452956-63-7

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	2940.00		NIST Webbook
rinpol	2940.00		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/molxK	981.10	Joback Method
cpg	991.52	J/molxK	1018.11	Joback Method
cpg	1001.92	J/molxK	1055.12	Joback Method
cpg	1010.60	J/molxK	1092.12	Joback Method
cpg	1017.53	J/molxK	1129.13	Joback Method
cpg	1022.70	J/molxK	1166.14	Joback Method
cpg	1026.08	J/molxK	1203.15	Joback Method

dvisc	0.0000495	Paxs	593.35	Joback Method
dvisc	0.0000234	Paxs	657.98	Joback Method
dvisc	0.0000126	Paxs	722.60	Joback Method
dvisc	0.0000075	Paxs	787.23	Joback Method
dvisc	0.0000049	Paxs	851.85	Joback Method
dvisc	0.0000033	Paxs	916.48	Joback Method
dvisc	0.0000024	Paxs	981.10	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=C452956637&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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