

4-((2R,3R,4R,5R)-3,4-Dimethyl-5-(3,4,5-trimethoxy

Inchi:	InChI=1S/C22H28O6/c1-12-13(2)21(15-10-18(25-4)22(27-6)19(11-15)26-5)28-20(12)14-
InchiKey:	XEDYWOVSWKYCOS-GETUCHRZSA-N
Formula:	C22H28O6
SMILES:	COc1cc(C2OC(c3cc(OC)c(OC)c(OC)c3)C(C)C2C)ccc1O
Mol. weight [g/mol]:	388.45
CAS:	114422-23-0

Physical Properties

Property code	Value	Unit	Source
gf	-326.66	kJ/mol	Joback Method
hf	-908.96	kJ/mol	Joback Method
hfus	54.92	kJ/mol	Joback Method
hvap	98.26	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.511		Crippen Method
mcvol	297.680	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	3003.90		NIST Webbook
rinpol	3003.90		NIST Webbook
tb	974.56	K	Joback Method
tc	1210.10	K	Joback Method
tf	666.01	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.27	J/molxK	974.56	Joback Method
cpg	1029.50	J/molxK	1013.82	Joback Method
cpg	1043.07	J/molxK	1053.07	Joback Method
cpg	1055.00	J/molxK	1092.33	Joback Method
cpg	1065.33	J/molxK	1131.58	Joback Method
cpg	1074.06	J/molxK	1170.84	Joback Method
cpg	1081.22	J/molxK	1210.10	Joback Method

dvisc	0.0000270	Paxs	666.01	Joback Method
dvisc	0.0000164	Paxs	717.43	Joback Method
dvisc	0.0000106	Paxs	768.86	Joback Method
dvisc	0.0000073	Paxs	820.29	Joback Method
dvisc	0.0000052	Paxs	871.71	Joback Method
dvisc	0.0000039	Paxs	923.13	Joback Method
dvisc	0.0000030	Paxs	974.56	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=C114422230&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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