4-Methoxy-6-((1S,3aR,4S,6aR)-4-(3,4,5-trimethoxy

Inchi: InChI=1S/C23H26O8/c1-24-16-5-12(6-17(25-2)22(16)27-4)20-14-9-29-21(15(14)10-28-2
InchiKey: DHWUVPPRBIJJKS-UHFFFAOYSA-N
Formula: C23H26O8
SMILES: COc1cc(C2OCC3C(c4cc(OC)c5c(c4)OCO5)OCC23)cc(OC)c1OC
Mol. weight [g/mol]: 430.45
CAS: 77394-27-5

Physical Properties

Property code	Value	Unit	Source
gf	-304.32	kJ/mol	Joback Method
hf	-984.95	kJ/mol	Joback Method
hfus	69.02	kJ/mol	Joback Method
hvap	102.77	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.525		Crippen Method
mcvol	301.790	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	3431.00		NIST Webbook
rinpol	3431.00		NIST Webbook
tb	1030.45	K	Joback Method
tc	1275.27	K	Joback Method
tf	714.67	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.08	J/mol×K	1030.45	Joback Method
cpg	1076.20	J/mol×K	1071.25	Joback Method
cpg	1087.61	J/mol×K	1112.06	Joback Method
cpg	1097.35	J/mol×K	1152.86	Joback Method
cpg	1105.48	J/mol×K	1193.66	Joback Method
cpg	1112.04	J/mol×K	1234.46	Joback Method
cpg	1117.08	J/mol×K	1275.27	Joback Method

dvisc	0.0008210	Pa×s	714.67	Joback Method
dvisc	0.0006607	Pa×s	767.30	Joback Method
dvisc	0.0005468	Pa×s	819.93	Joback Method
dvisc	0.0004629	Pa×s	872.56	Joback Method
dvisc	0.0003994	Pa×s	925.19	Joback Method
dvisc	0.0003502	Pa×s	977.82	Joback Method
dvisc	0.0003111	Pa×s	1030.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77394275&Units=SI
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

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