5-((1S,3aR,4S,6aR)-4-(3,4,5-Trimethoxyphenyl)hex

Inchi: InChI=1S/C22H24O7/c1-23-18-7-13(8-19(24-2)22(18)25-3)21-15-10-26-20(14(15)9-27-2
InchiKey: ONDWGDNAFRAXCN-UHFFFAOYSA-N
Formula: C22H24O7
SMILES: COc1cc(C2OCC3C(c4ccc5c(c4)OCO5)OCC23)cc(OC)c1OC
Mol. weight [g/mol]: 400.42
CAS: 13060-15-6

Physical Properties

Property code	Value	Unit	Source
gf	-198.11	kJ/mol	Joback Method
hf	-820.62	kJ/mol	Joback Method
hfus	65.63	kJ/mol	Joback Method
hvap	97.47	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.516		Crippen Method
mcvol	281.830	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	3212.80		NIST Webbook
rinpol	3212.80		NIST Webbook
tb	980.17	K	Joback Method
tc	1225.64	K	Joback Method
tf	668.65	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.78	J/mol×K	980.17	Joback Method
cpg	992.46	J/mol×K	1021.08	Joback Method
cpg	1005.64	J/mol×K	1061.99	Joback Method
cpg	1017.40	J/mol×K	1102.90	Joback Method
cpg	1027.80	J/mol×K	1143.81	Joback Method
cpg	1036.94	J/mol×K	1184.72	Joback Method
cpg	1044.88	J/mol×K	1225.64	Joback Method

dvisc	0.0012124	Pa×s	668.65	Joback Method
dvisc	0.0009671	Pa×s	720.57	Joback Method
dvisc	0.0007952	Pa×s	772.49	Joback Method
dvisc	0.0006702	Pa×s	824.41	Joback Method
dvisc	0.0005764	Pa×s	876.33	Joback Method
dvisc	0.0005042	Pa×s	928.25	Joback Method
dvisc	0.0004473	Pa×s	980.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13060156&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

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