(2S,3S,4S,5S)-2-(3,4-Dimethoxyphenyl)-3,4-dimeth

Inchi: InChI=1S/C23H30O6/c1-13-14(2)22(16-11-19(26-5)23(28-7)20(12-16)27-6)29-21(13)15-

InchiKey: FUFHSLKNBJRCDG-LPINMEDASA-N

Formula: C23H30O6

SMILES: COc1ccc(C2OC(c3cc(OC)c(OC)c(OC)c3)C(C)C2C)cc1OC

Mol. weight [g/mol]: 402.48

CAS: 184486-87-1

Physical Properties

Property code	Value	Unit	Source
gf	-278.25	kJ/mol	Joback Method
hf	-895.98	kJ/mol	Joback Method
hfus	52.53	kJ/mol	Joback Method
hvap	90.54	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.814		Crippen Method
mcvol	311.770	ml/mol	McGowan Method
pc	1229.42	kPa	Joback Method
rinpol	3016.00		NIST Webbook
rinpol	3016.00		NIST Webbook
tb	944.22	K	Joback Method
tc	1170.35	K	Joback Method
tf	600.31	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1046.72	J/mol×K	944.22	Joback Method
cpg	1062.26	J/mol×K	981.91	Joback Method
cpg	1075.65	J/mol×K	1019.60	Joback Method
cpg	1086.86	J/mol×K	1057.28	Joback Method
cpg	1095.83	J/mol×K	1094.97	Joback Method
cpg	1102.51	J/mol×K	1132.66	Joback Method
cpg	1106.88	J/mol×K	1170.35	Joback Method

dvisc	0.0002194	Pa×s	600.31	Joback Method
dvisc	0.0001573	Pa×s	657.63	Joback Method
dvisc	0.0001190	Pa×s	714.95	Joback Method
dvisc	0.0000938	Pa×s	772.27	Joback Method
dvisc	0.0000764	Pa×s	829.58	Joback Method
dvisc	0.0000639	Pa×s	886.90	Joback Method
dvisc	0.0000546	Pa×s	944.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C184486871&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