(2R,4R,5S)-2,4-bis(4-Methoxyphenyl)-5-methyl-1,3

Inchi: InChI=1S/C18H20O4/c1-12-17(13-4-8-15(19-2)9-5-13)22-18(21-12)14-6-10-16(20-3)11-7

InchiKey: LYZZEJQTEOAYRE-UHFFFAOYSA-N

Formula: C18H20O4

SMILES: COc1ccc(C2OC(C)C(c3ccc(OC)cc3)O2)cc1

Mol. weight [g/mol]: 300.35

CAS: 212516-36-4

Physical Properties

Property code	Value	Unit	Source
gf	-54.87	kJ/mol	Joback Method
hf	-473.37	kJ/mol	Joback Method
hfus	44.09	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.879		Crippen Method
mcvol	229.580	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2452.90		NIST Webbook
rinpol	2452.90		NIST Webbook
tb	779.24	K	Joback Method
tc	1018.61	K	Joback Method
tf	470.52	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.85	J/mol×K	779.24	Joback Method
cpg	714.16	J/mol×K	819.13	Joback Method
cpg	730.88	J/mol×K	859.03	Joback Method
cpg	746.02	J/mol×K	898.92	Joback Method
cpg	759.61	J/mol×K	938.82	Joback Method
cpg	771.67	J/mol×K	978.71	Joback Method
cpg	782.23	J/mol×K	1018.61	Joback Method

dvisc	0.0008089	Pa×s	470.52	Joback Method
dvisc	0.0005228	Pa×s	521.97	Joback Method
dvisc	0.0003655	Pa×s	573.43	Joback Method
dvisc	0.0002710	Pa×s	624.88	Joback Method
dvisc	0.0002103	Pa×s	676.33	Joback Method
dvisc	0.0001691	Pa×s	727.79	Joback Method
dvisc	0.0001400	Pa×s	779.24	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=C212516364&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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