(2R,3S,5S,6R)-2,5-bis(4-Methoxyphenyl)-3,6-dimet

Inchi: InChI=1S/C20H24O4/c1-13-19(15-5-9-17(21-3)10-6-15)24-14(2)20(23-13)16-7-11-18(22
InchiKey: TWEGIGPRPZZEHS-UHFFFAOYSA-N
Formula: C20H24O4
SMILES: COc1ccc(C2OC(C)C(c3ccc(OC)cc3)OC2C)cc1
Mol. weight [g/mol]: 328.40
CAS: 212516-42-2

Physical Properties

Property code	Value	Unit	Source
gf	-57.84	kJ/mol	Joback Method
hf	-541.15	kJ/mol	Joback Method
hfus	48.24	kJ/mol	Joback Method
hvap	79.33	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.310		Crippen Method
mcvol	257.760	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	2566.80		NIST Webbook
rinpol	2566.80		NIST Webbook
tb	824.60	K	Joback Method
tc	1062.24	K	Joback Method
tf	485.30	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.48	J/mol×K	824.60	Joback Method
cpg	895.61	J/mol×K	1022.63	Joback Method
cpg	883.85	J/mol×K	983.03	Joback Method
cpg	870.26	J/mol×K	943.42	Joback Method
cpg	854.85	J/mol×K	903.81	Joback Method
cpg	837.59	J/mol×K	864.21	Joback Method
cpg	905.56	J/mol×K	1062.24	Joback Method

dvisc	0.0000998	Pa×s	824.60	Joback Method
dvisc	0.0001218	Pa×s	768.05	Joback Method
dvisc	0.0001535	Pa×s	711.50	Joback Method
dvisc	0.0002014	Pa×s	654.95	Joback Method
dvisc	0.0002782	Pa×s	598.40	Joback Method
dvisc	0.0004109	Pa×s	541.85	Joback Method
dvisc	0.0006648	Pa×s	485.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C212516422&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