(1R,2S,3R)-1,4-Bis(benzo[d][1,3]dioxol-5-yl)-2,3-di

Inchi: InChI=1S/C20H22O5/c1-12(7-14-3-5-16-18(8-14)24-10-22-16)13(2)20(21)15-4-6-17-19(9
InchiKey: SDXLCXZRXWWAGW-UHFFFAOYSA-N
Formula: C20H22O5
SMILES: CC(Cc1ccc2c(c1)OCO2)C(C)C(O)c1ccc2c(c1)OCO2
Mol. weight [g/mol]: 342.39
CAS: 111786-59-5

Physical Properties

Property code	Value	Unit	Source
gf	-47.88	kJ/mol	Joback Method
hf	-538.74	kJ/mol	Joback Method
hfus	53.65	kJ/mol	Joback Method
hvap	101.31	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	3.692		Crippen Method
mcvol	252.770	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinpol	2779.50		NIST Webbook
rinpol	2779.50		NIST Webbook
tb	951.76	K	Joback Method
tc	1185.39	K	Joback Method
tf	584.54	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.87	J/mol×K	951.76	Joback Method
cpg	843.33	J/mol×K	990.70	Joback Method
cpg	856.23	J/mol×K	1029.64	Joback Method
cpg	868.72	J/mol×K	1068.58	Joback Method
cpg	880.93	J/mol×K	1107.52	Joback Method
cpg	893.01	J/mol×K	1146.46	Joback Method
cpg	905.10	J/mol×K	1185.39	Joback Method

dvisc	0.0006363	Pa×s	584.54	Joback Method
dvisc	0.0003189	Pa×s	645.74	Joback Method
dvisc	0.0001802	Pa×s	706.95	Joback Method
dvisc	0.0001115	Pa×s	768.15	Joback Method
dvisc	0.0000740	Pa×s	829.35	Joback Method
dvisc	0.0000520	Pa×s	890.56	Joback Method
dvisc	0.0000382	Pa×s	951.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111786595&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