(2R,3R)-2,3-bis(Benzo[d][1,3]dioxol-5-ylmethyl)bu

Inchi: InChI=1S/C20H22O6/c21-9-15(5-13-1-3-17-19(7-13)25-11-23-17)16(10-22)6-14-2-4-18-2
InchiKey: JKCVMTYNARDGET-HZPDHXFCSA-N
Formula: C20H22O6
SMILES: OCC(Cc1ccc2c(c1)OCO2)C(CO)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 358.39
CAS: 24563-03-9

Physical Properties

Property code	Value	Unit	Source
gf	-182.26	kJ/mol	Joback Method
hf	-685.69	kJ/mol	Joback Method
hfus	61.26	kJ/mol	Joback Method
hvap	118.38	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	2.146		Crippen Method
mcvol	258.640	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	3182.40		NIST Webbook
tb	1044.38	K	Joback Method
tc	1280.19	K	Joback Method
tf	660.36	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.35	J/mol×K	1044.38	Joback Method
cpg	892.02	J/mol×K	1083.68	Joback Method
cpg	904.50	J/mol×K	1122.98	Joback Method
cpg	916.93	J/mol×K	1162.28	Joback Method
cpg	929.45	J/mol×K	1201.59	Joback Method
cpg	942.23	J/mol×K	1240.89	Joback Method
cpg	955.42	J/mol×K	1280.19	Joback Method
dvisc	0.0001225	Pa×s	660.36	Joback Method

dvisc	0.0000553	Pa×s	724.36	Joback Method
dvisc	0.0000284	Pa×s	788.37	Joback Method
dvisc	0.0000161	Pa×s	852.37	Joback Method
dvisc	0.0000099	Pa×s	916.37	Joback Method
dvisc	0.0000065	Pa×s	980.38	Joback Method
dvisc	0.0000045	Pa×s	1044.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24563039&Units=SI

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