5,5'-((2R,3S)-2,3-Dimethylbutane-1,4-diyl)bis(benz

Inchi: InChI=1S/C20H22O4/c1-13(7-15-3-5-17-19(9-15)23-11-21-17)14(2)8-16-4-6-18-20(10-16
InchiKey: QEFJURUMSHPMTC-UHFFFAOYSA-N
Formula: C20H22O4
SMILES: CC(Cc1ccc2c(c1)OCO2)C(C)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 326.39
CAS: 110269-50-6

Physical Properties

Property code	Value	Unit	Source
gf	91.38	kJ/mol	Joback Method
hf	-381.23	kJ/mol	Joback Method
hfus	53.08	kJ/mol	Joback Method
hvap	85.02	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.201		Crippen Method
mcvol	246.900	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2598.30		NIST Webbook
rinpol	2598.30		NIST Webbook
tb	860.02	K	Joback Method
tc	1101.32	K	Joback Method
tf	538.72	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.12	J/mol×K	860.02	Joback Method
cpg	847.12	J/mol×K	1061.11	Joback Method
cpg	834.16	J/mol×K	1020.89	Joback Method
cpg	820.73	J/mol×K	980.67	Joback Method
cpg	806.69	J/mol×K	940.45	Joback Method
cpg	791.87	J/mol×K	900.24	Joback Method
cpg	859.78	J/mol×K	1101.32	Joback Method

dvisc	0.0002992	Pa×s	860.02	Joback Method
dvisc	0.0003630	Pa×s	806.47	Joback Method
dvisc	0.0004526	Pa×s	752.92	Joback Method
dvisc	0.0005838	Pa×s	699.37	Joback Method
dvisc	0.0007854	Pa×s	645.82	Joback Method
dvisc	0.0011148	Pa×s	592.27	Joback Method
dvisc	0.0016967	Pa×s	538.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110269506&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