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

Inchi: InChI=1S/C20H26O4/c1-13(9-15-5-7-17(21)19(11-15)23-3)14(2)10-16-6-8-18(22)20(12-1
InchiKey: ADFOLUXMYYCTRR-UHFFFAOYSA-N
Formula: C20H26O4
SMILES: COc1cc(CC(C)C(C)Cc2ccc(O)c(OC)c2)ccc1O
Mol. weight [g/mol]: 330.42
CAS: 66322-34-7

Physical Properties

Property code	Value	Unit	Source
gf	-201.04	kJ/mol	Joback Method
hf	-635.63	kJ/mol	Joback Method
hfus	41.76	kJ/mol	Joback Method
hvap	96.06	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.172		Crippen Method
mcvol	268.620	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	2714.60		NIST Webbook
rinpol	2714.60		NIST Webbook
tb	925.52	K	Joback Method
tc	1160.51	K	Joback Method
tf	630.94	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.72	J/mol×K	925.52	Joback Method
cpg	937.29	J/mol×K	1121.34	Joback Method
cpg	922.52	J/mol×K	1082.18	Joback Method
cpg	907.62	J/mol×K	1043.01	Joback Method
cpg	892.44	J/mol×K	1003.85	Joback Method
cpg	876.86	J/mol×K	964.68	Joback Method
cpg	952.05	J/mol×K	1160.51	Joback Method

dvisc	8.0544022e-08	Pa×s	925.52	Joback Method
dvisc	0.0000001	Pa×s	876.42	Joback Method
dvisc	0.0000002	Pa×s	827.33	Joback Method
dvisc	0.0000004	Pa×s	778.23	Joback Method
dvisc	0.0000007	Pa×s	729.13	Joback Method
dvisc	0.0000015	Pa×s	680.04	Joback Method
dvisc	0.0000035	Pa×s	630.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66322347&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