1,3-Benzodioxole, 5,5'-(tetrahydro-1H,3H-furo[3,4-c]furan-1,4-diyl)bis (1S,3aR,4S,6aR)-

Other names: sesamin

IUPAC Name: (1S,3aR,4S,6aR)-1,4-Bis(benzo[d][1,3]dioxol-5-yl)hexahydrofuro[3,4-c]furan

Inchi: InChI=1S/C20H18O6/c1-3-15-17(25-9-23-15)5-11(1)19-13-7-22-20(14(13)8-21-19)12-2-4

InchiKey: PEYUIKBAABKQKQ-UHFFFAOYSA-N

Formula: C20H18O6

SMILES: c1cc2c(cc1C1OCC3C(c4ccc5c(c4)OCO5)OCC13)OCO2

Mol. weight [g/mol]: 354.35

CAS: 607-80-7

Physical Properties

Property code	Value	Unit	Source
gf	5.90	kJ/mol	Joback Method
hf	-542.07	kJ/mol	Joback Method
hfus	70.30	kJ/mol	Joback Method
hvap	94.37	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.219		Crippen Method
mcvol	236.920	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	3150.90		NIST Webbook
rinpol	3150.90		NIST Webbook
tb	927.48	K	Joback Method
tc	1193.90	K	Joback Method
tf	642.22	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.93	J/mol×K	927.48	Joback Method
cpg	831.91	J/mol×K	971.88	Joback Method
cpg	847.04	J/mol×K	1016.29	Joback Method
cpg	861.58	J/mol×K	1060.69	Joback Method
cpg	875.78	J/mol×K	1105.10	Joback Method

cpg	889.86	J/mol×K	1149.50	Joback Method
cpg	904.09	J/mol×K	1193.90	Joback Method
dvisc	0.0054836	Pa×s	642.22	Joback Method
dvisc	0.0045300	Pa×s	689.76	Joback Method
dvisc	0.0038355	Pa×s	737.31	Joback Method
dvisc	0.0033137	Pa×s	784.85	Joback Method
dvisc	0.0029111	Pa×s	832.39	Joback Method
dvisc	0.0025934	Pa×s	879.94	Joback Method
dvisc	0.0023380	Pa×s	927.48	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C607807&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

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