(3R,4R)-3-(Benzo[d][1,3]dioxol-5-ylmethyl)-4-(3,4-d

Inchi: InChI=1S/C21H22O6/c1-23-17-5-3-13(9-19(17)24-2)7-15-11-25-21(22)16(15)8-14-4-6-18

InchiKey: LEVKKQBBEVGIKN-CVEARBPZSA-N

Formula: C21H22O6

SMILES: COc1ccc(CC2COC(=O)C2Cc2ccc3c(c2)OCO3)cc1OC

Mol. weight [g/mol]: 370.40

CAS: 58311-20-9

Physical Properties

Property code	Value	Unit	Source
gf	-181.41	kJ/mol	Joback Method
hf	-714.45	kJ/mol	Joback Method
hfus	54.57	kJ/mol	Joback Method
hvap	92.31	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.007		Crippen Method
mcvol	268.430	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	3109.20		NIST Webbook
rinpol	3109.20		NIST Webbook
tb	968.69	K	Joback Method
tc	1217.59	K	Joback Method
tf	650.58	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.82	J/mol×K	968.69	Joback Method
cpg	914.42	J/mol×K	1010.17	Joback Method
cpg	926.27	J/mol×K	1051.66	Joback Method
cpg	936.41	J/mol×K	1093.14	Joback Method
cpg	944.85	J/mol×K	1134.63	Joback Method
cpg	951.64	J/mol×K	1176.11	Joback Method
cpg	956.82	J/mol×K	1217.59	Joback Method

Sources

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=C58311209&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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