(3R,4R)-3-((7-Methoxybenzo[d][1,3]dioxol-5-yl)me

Inchi: InChI=1S/C23H26O8/c1-25-17-7-13(8-18(26-2)21(17)28-4)5-15-11-29-23(24)16(15)6-14
InchiKey: BFDODNWEBMWJIS-CVEARBPZSA-N
Formula: C23H26O8
SMILES: COc1cc(CC2COC(=O)C2Cc2cc(OC)c3c(c2)OCO3)cc(OC)c1OC
Mol. weight [g/mol]: 430.45
CAS: 101751-71-7

Physical Properties

Property code	Value	Unit	Source
gf	-393.83	kJ/mol	Joback Method
hf	-1043.11	kJ/mol	Joback Method
hfus	61.34	kJ/mol	Joback Method
hvap	102.90	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.024		Crippen Method
mcvol	308.350	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	3402.50		NIST Webbook
rinpol	3402.50		NIST Webbook
tb	1069.25	K	Joback Method
tc	1317.35	K	Joback Method
tf	742.62	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.31	J/mol×K	1069.25	Joback Method
cpg	1075.71	J/mol×K	1110.60	Joback Method
cpg	1082.75	J/mol×K	1151.95	Joback Method
cpg	1087.41	J/mol×K	1193.30	Joback Method
cpg	1089.66	J/mol×K	1234.65	Joback Method
cpg	1089.47	J/mol×K	1276.00	Joback Method
cpg	1086.84	J/mol×K	1317.35	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=C101751717&Units=SI

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