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

Inchi: InChI=1S/C22H24O7/c1-24-19-9-14(10-20(25-2)21(19)26-3)7-16-15(11-27-22(16)23)6-1
InchiKey: GMLDZDDTZKXJLU-CVEARBPZSA-N
Formula: C22H24O7
SMILES: COc1cc(CC2C(=O)OCC2Cc2ccc3c(c2)OCO3)cc(OC)c1OC
Mol. weight [g/mol]: 400.42
CAS: 40456-50-6

Physical Properties

Property code	Value	Unit	Source
gf	-287.62	kJ/mol	Joback Method
hf	-878.78	kJ/mol	Joback Method
hfus	57.95	kJ/mol	Joback Method
hvap	97.61	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.015		Crippen Method
mcvol	288.390	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	3225.80		NIST Webbook
tb	1018.97	K	Joback Method
tc	1265.82	K	Joback Method
tf	696.60	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.41	J/mol×K	1018.97	Joback Method
cpg	996.20	J/mol×K	1060.11	Joback Method
cpg	1005.99	J/mol×K	1101.25	Joback Method
cpg	1013.79	J/mol×K	1142.39	Joback Method
cpg	1019.61	J/mol×K	1183.53	Joback Method
cpg	1023.44	J/mol×K	1224.68	Joback Method
cpg	1025.30	J/mol×K	1265.82	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=C40456506&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