(3R,4R)-4-(3,4-Dimethoxybenzyl)-3-(3,4,5-trimetho

Inchi: InChI=1S/C23H28O7/c1-25-18-7-6-14(10-19(18)26-2)8-16-13-30-23(24)17(16)9-15-11-2
InchiKey: QFFURUDOUPSWTF-SJORKVTESA-N
Formula: C23H28O7
SMILES: COc1ccc(CC2COC(=O)C2Cc2cc(OC)c(OC)c(OC)c2)cc1OC
Mol. weight [g/mol]: 416.46
CAS: 10516-73-1

Physical Properties

Property code	Value	Unit	Source
gf	-385.42	kJ/mol	Joback Method
hf	-993.00	kJ/mol	Joback Method
hfus	49.90	kJ/mol	Joback Method
hvap	95.41	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.304		Crippen Method
mcvol	313.340	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	3234.30		NIST Webbook
rinpol	3234.30		NIST Webbook
tb	1021.38	K	Joback Method
tc	1259.48	K	Joback Method
tf	677.01	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1061.63	J/mol×K	1021.38	Joback Method
cpg	1072.38	J/mol×K	1061.06	Joback Method
cpg	1080.50	J/mol×K	1100.75	Joback Method
cpg	1085.91	J/mol×K	1140.43	Joback Method
cpg	1088.54	J/mol×K	1180.11	Joback Method
cpg	1088.32	J/mol×K	1219.80	Joback Method
cpg	1085.18	J/mol×K	1259.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10516731&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
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