Benzoic acid 4,5-dimethoxy-2-methoxy methyl-tetrahydro-pyran-3-yl ester

Inchi: InChI=1S/C16H22O6/c1-18-9-11-7-14(19-2)15(20-3)8-13(11)16(17)22-12-5-4-6-21-10-12

InchiKey: ZSWIENPEDRKNNH-UHFFFAOYSA-N

Formula: C16H22O6

SMILES: COCc1cc(OC)c(OC)cc1C(=O)OC1CCCOC1

Mol. weight [g/mol]: 310.34

Physical Properties

Property code	Value	Unit	Source
gf	-443.23	kJ/mol	Joback Method
hf	-890.59	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.186		Crippen Method
mcvol	232.600	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	2073.71		NIST Webbook
rinpol	2034.39		NIST Webbook
tb	797.15	K	Joback Method
tc	1016.48	K	Joback Method
tf	506.86	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.15	J/mol×K	797.15	Joback Method
cpg	727.68	J/mol×K	833.70	Joback Method
cpg	742.81	J/mol×K	870.26	Joback Method
cpg	756.50	J/mol×K	906.81	Joback Method
cpg	768.74	J/mol×K	943.37	Joback Method
cpg	779.49	J/mol×K	979.92	Joback Method
cpg	788.72	J/mol×K	1016.48	Joback Method
dvisc	0.0003801	Pa×s	506.86	Joback Method

dvisc	0.0002356	Pa×s	555.24	Joback Method
dvisc	0.0001577	Pa×s	603.62	Joback Method
dvisc	0.0001120	Pa×s	652.00	Joback Method
dvisc	0.0000834	Pa×s	700.39	Joback Method
dvisc	0.0000645	Pa×s	748.77	Joback Method
dvisc	0.0000515	Pa×s	797.15	Joback Method

Sources

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=R273724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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