Benzoic acid 4,5-diethoxy-2-ethoxymethyl-tetrahydro-pyran-3-yl ester

Inchi: InChI=1S/C19H28O6/c1-4-21-12-14-10-17(23-5-2)18(24-6-3)11-16(14)19(20)25-15-8-7-9

InchiKey: UPMIGZRNITUKAA-UHFFFAOYSA-N

Formula: C19H28O6

SMILES: CCOCc1cc(OCC)c(OCC)cc1C(=O)OC1CCCOC1

Mol. weight [g/mol]: 352.42

Physical Properties

Property code	Value	Unit	Source
gf	-417.97	kJ/mol	Joback Method
hf	-952.51	kJ/mol	Joback Method
hfus	44.00	kJ/mol	Joback Method
hvap	83.47	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.356		Crippen Method
mcvol	274.870	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2164.99		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	865.79	K	Joback Method
tc	1080.24	K	Joback Method
tf	540.67	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.89	J/mol×K	865.79	Joback Method
cpg	902.34	J/mol×K	901.53	Joback Method
cpg	917.22	J/mol×K	937.27	Joback Method
cpg	930.53	J/mol×K	973.01	Joback Method
cpg	942.25	J/mol×K	1008.76	Joback Method
cpg	952.35	J/mol×K	1044.50	Joback Method
cpg	960.82	J/mol×K	1080.24	Joback Method
dvisc	0.0002843	Pa×s	540.67	Joback Method

dvisc	0.0001696	Pa×s	594.86	Joback Method
dvisc	0.0001103	Pa×s	649.04	Joback Method
dvisc	0.0000767	Pa×s	703.23	Joback Method
dvisc	0.0000561	Pa×s	757.42	Joback Method
dvisc	0.0000428	Pa×s	811.60	Joback Method
dvisc	0.0000338	Pa×s	865.79	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R273704&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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