Benzoic acid, 4-pentyloxy-, pentyl ester

Inchi: InChI=1S/C17H26O3/c1-3-5-7-13-19-16-11-9-15(10-12-16)17(18)20-14-8-6-4-2/h9-12H,3
InchiKey: LINWQIFFERKCKA-UHFFFAOYSA-N
Formula: C17H26O3
SMILES: CCCCCOC(=O)c1ccc(OCCCCC)cc1
Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
gf	-143.88	kJ/mol	Joback Method
hf	-546.17	kJ/mol	Joback Method
hfus	37.41	kJ/mol	Joback Method
hvap	67.94	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.603		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
rinpol	2162.00		NIST Webbook
tb	718.73	K	Joback Method
tc	912.24	K	Joback Method
tf	414.68	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.80	J/mol×K	718.73	Joback Method
cpg	700.78	J/mol×K	750.98	Joback Method
cpg	716.81	J/mol×K	783.23	Joback Method
cpg	731.90	J/mol×K	815.49	Joback Method
cpg	746.06	J/mol×K	847.74	Joback Method
cpg	759.31	J/mol×K	879.99	Joback Method
cpg	771.65	J/mol×K	912.24	Joback Method
dvisc	0.0009484	Pa×s	414.68	Joback Method
dvisc	0.0005072	Pa×s	465.36	Joback Method

dvisc	0.0003067	Pa×s	516.03	Joback Method
dvisc	0.0002029	Pa×s	566.71	Joback Method
dvisc	0.0001437	Pa×s	617.38	Joback Method
dvisc	0.0001072	Pa×s	668.06	Joback Method
dvisc	0.0000834	Pa×s	718.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374560&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