

Benzoic acid, 3-pentyloxy-, pentyl ester

Inchi:	InChI=1S/C17H26O3/c1-3-5-7-12-19-16-11-9-10-15(14-16)17(18)20-13-8-6-4-2/h9-11,14
InchiKey:	GQTVLGIAYIACHZ-UHFFFAOYSA-N
Formula:	C17H26O3
SMILES:	CCCCCOC(=O)c1cccc(OCCCC)c1
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
rinsol	2092.00		NIST Webbook
tb	718.73	K	Joback Method
tc	912.24	K	Joback Method
tf	414.68	K	Joback Method
vc	0.921	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003067	Paxs	516.03	Joback Method
dvisc	0.0002029	Paxs	566.71	Joback Method
dvisc	0.0001437	Paxs	617.38	Joback Method
dvisc	0.0001072	Paxs	668.06	Joback Method
dvisc	0.0000834	Paxs	718.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374562&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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

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