

2-(Benzoyloxy)propyl benzoate

Inchi:	InChI=1S/C17H16O4/c1-13(21-17(19)15-10-6-3-7-11-15)12-20-16(18)14-8-4-2-5-9-14/h2
InchiKey:	UMVMVEZHMZTUHD-UHFFFAOYSA-N
Formula:	C17H16O4
SMILES:	CC(COC(=O)c1ccccc1)OC(=O)c1ccccc1
Mol. weight [g/mol]:	284.31

Physical Properties

Property code	Value	Unit	Source
gf	-153.20	kJ/mol	Joback Method
hf	-416.03	kJ/mol	Joback Method
hfus	29.92	kJ/mol	Joback Method
hvap	75.91	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.089		Crippen Method
mcvol	217.750	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
tb	793.86	K	Joback Method
tc	1029.01	K	Joback Method
tf	463.51	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.70	J/molxK	793.86	Joback Method
cpg	628.81	J/molxK	833.05	Joback Method
cpg	641.63	J/molxK	872.24	Joback Method
cpg	653.19	J/molxK	911.43	Joback Method
cpg	663.54	J/molxK	950.63	Joback Method
cpg	672.71	J/molxK	989.82	Joback Method
cpg	680.74	J/molxK	1029.01	Joback Method
dvisc	0.0009003	Paxs	463.51	Joback Method
dvisc	0.0004793	Paxs	518.57	Joback Method
dvisc	0.0002880	Paxs	573.63	Joback Method

dvisc	0.0001892	Paxs	628.69	Joback Method
dvisc	0.0001330	Paxs	683.74	Joback Method
dvisc	0.0000985	Paxs	738.80	Joback Method
dvisc	0.0000761	Paxs	793.86	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009454&Units=SI

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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