1-Propanol, 2-[2-(benzoyloxy)propoxy]-, benzoate

Other names: Dipropyleneglycol dibenzoate
2-[2-(benzoyloxy)propoxy]propyl benzoate
Inchi: InChI=1S/C20H22O5/c1-15(13-24-19(21)17-9-5-3-6-10-17)23-14-16(2)25-20(22)18-11-7
InchiKey: LXODQLXKQIJVNK-UHFFFAOYSA-N
Formula: C20H22O5
SMILES: CC(COC(=O)c1ccccc1)OCC(C)OC(=O)c1ccccc1
Mol. weight [g/mol]: 342.39
CAS: 20109-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-235.38	kJ/mol	Joback Method
hf	-615.45	kJ/mol	Joback Method
hfus	35.35	kJ/mol	Joback Method
hvap	84.61	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.494		Crippen Method
mcvol	265.890	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
tb	884.48	K	Joback Method
tc	1112.15	K	Joback Method
tf	504.55	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.98	J/mol×K	884.48	Joback Method
cpg	866.15	J/mol×K	1074.21	Joback Method
cpg	857.88	J/mol×K	1036.26	Joback Method
cpg	848.26	J/mol×K	998.32	Joback Method
cpg	837.25	J/mol×K	960.37	Joback Method
cpg	824.84	J/mol×K	922.43	Joback Method
cpg	873.09	J/mol×K	1112.15	Joback Method

dvisc	0.0000347	Pa×s	884.48	Joback Method
dvisc	0.0000458	Pa×s	821.16	Joback Method
dvisc	0.0000634	Pa×s	757.84	Joback Method
dvisc	0.0000931	Pa×s	694.51	Joback Method
dvisc	0.0001477	Pa×s	631.19	Joback Method
dvisc	0.0002596	Pa×s	567.87	Joback Method
dvisc	0.0005260	Pa×s	504.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20109391&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume