1,2-Diacetoxy-3-[2-(3-phenylpropionyl)phenoxy]p

Other names: Propafenone desamino hydroxy, acetylated
Inchi: InChI=1S/C22H24O6/c1-16(23)26-14-19(28-17(2)24)15-27-22-11-7-6-10-20(22)21(25)13
InchiKey: BIOFQKZXILPLAT-UHFFFAOYSA-N
Formula: C22H24O6
SMILES: CC(=O)OCC(COc1ccccc1C(=O)CCc1ccccc1)OC(C)=O
Mol. weight [g/mol]: 384.42

Physical Properties

Property code	Value	Unit	Source
gf	-354.65	kJ/mol	Joback Method
hf	-775.50	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	96.86	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.376		Crippen Method
mcvol	295.640	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	2715.00		NIST Webbook
rinpol	2715.00		NIST Webbook
tb	989.53	K	Joback Method
tc	1221.32	K	Joback Method
tf	604.54	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.16	J/mol×K	989.53	Joback Method
cpg	945.31	J/mol×K	1028.16	Joback Method
cpg	954.90	J/mol×K	1066.79	Joback Method
cpg	962.97	J/mol×K	1105.43	Joback Method
cpg	969.54	J/mol×K	1144.06	Joback Method
cpg	974.65	J/mol×K	1182.69	Joback Method
cpg	978.31	J/mol×K	1221.32	Joback Method

dvisc	0.0002662	Pa×s	604.54	Joback Method
dvisc	0.0001518	Pa×s	668.70	Joback Method
dvisc	0.0000955	Pa×s	732.87	Joback Method
dvisc	0.0000647	Pa×s	797.03	Joback Method
dvisc	0.0000465	Pa×s	861.20	Joback Method
dvisc	0.0000350	Pa×s	925.37	Joback Method
dvisc	0.0000273	Pa×s	989.53	Joback Method

Sources

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=U281338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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