Benzoic acid, 2-(1-phenylethyl)-4-methoxyphenyl ester

Inchi: InChI=1S/C22H20O3/c1-16(17-9-5-3-6-10-17)20-15-19(24-2)13-14-21(20)25-22(23)18-1

InchiKey: VHBZEMZRVWNDBY-UHFFFAOYSA-N

Formula: C22H20O3

SMILES: COc1ccc(OC(=O)c2ccccc2)c(C(C)c2ccccc2)c1

Mol. weight [g/mol]: 332.39

Physical Properties

Property code	Value	Unit	Source
gf	110.97	kJ/mol	Joback Method
hf	-193.06	kJ/mol	Joback Method
hfus	34.53	kJ/mol	Joback Method
hvap	83.90	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.066		Crippen Method
mcvol	262.870	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
rinpol	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	891.03	K	Joback Method
tc	1140.32	K	Joback Method
tf	521.39	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.17	J/mol×K	891.03	Joback Method
cpg	798.79	J/mol×K	932.58	Joback Method
cpg	811.85	J/mol×K	974.13	Joback Method
cpg	823.42	J/mol×K	1015.67	Joback Method
cpg	833.57	J/mol×K	1057.22	Joback Method
cpg	842.35	J/mol×K	1098.77	Joback Method
cpg	849.85	J/mol×K	1140.32	Joback Method
dvisc	0.0004275	Pa×s	521.39	Joback Method

dvisc	0.0002371	Pa×s	583.00	Joback Method
dvisc	0.0001472	Pa×s	644.60	Joback Method
dvisc	0.0000993	Pa×s	706.21	Joback Method
dvisc	0.0000714	Pa×s	767.82	Joback Method
dvisc	0.0000539	Pa×s	829.42	Joback Method
dvisc	0.0000423	Pa×s	891.03	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=U360149&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume