3-Chlorobenzoic acid, 2-(1-phenylethyl)-4-methoxyphenyl ester

Inchi: InChI=1S/C22H19ClO3/c1-15(16-7-4-3-5-8-16)20-14-19(25-2)11-12-21(20)26-22(24)17-9

InchiKey: IAVPSAAYWBLORH-UHFFFAOYSA-N

Formula: C22H19ClO3

SMILES: COc1ccc(OC(=O)c2cccc(Cl)c2)c(C(C)c2ccccc2)c1

Mol. weight [g/mol]: 366.84

Physical Properties

Property code	Value	Unit	Source
gf	89.41	kJ/mol	Joback Method
hf	-220.27	kJ/mol	Joback Method
hfus	38.34	kJ/mol	Joback Method
hvap	88.94	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.720		Crippen Method
mcvol	275.110	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	2794.00		NIST Webbook
rinpol	2794.00		NIST Webbook
tb	933.44	K	Joback Method
tc	1185.53	K	Joback Method
tf	563.83	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.78	J/mol×K	933.44	Joback Method
cpg	854.51	J/mol×K	1143.52	Joback Method
cpg	847.36	J/mol×K	1101.50	Joback Method
cpg	838.88	J/mol×K	1059.49	Joback Method
cpg	829.00	J/mol×K	1017.47	Joback Method
cpg	817.65	J/mol×K	975.46	Joback Method
cpg	860.39	J/mol×K	1185.53	Joback Method
dvisc	0.0000375	Pa×s	933.44	Joback Method

dvisc	0.0000471	Pa×s	871.84	Joback Method
dvisc	0.0000613	Pa×s	810.24	Joback Method
dvisc	0.0000834	Pa×s	748.63	Joback Method
dvisc	0.0001199	Pa×s	687.03	Joback Method
dvisc	0.0001851	Pa×s	625.43	Joback Method
dvisc	0.0003141	Pa×s	563.83	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=U360146&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