Benzoic acid, 2-chloro-, 4-benzyloxyphenyl ester

Other names: 2-Chlorobenzoic acid, 4-benzyloxyphenyl ester
Inchi: InChI=1S/C20H15ClO3/c21-19-9-5-4-8-18(19)20(22)24-17-12-10-16(11-13-17)23-14-15-
InchiKey: UQSRIVDYEKEWHD-UHFFFAOYSA-N
Formula: C20H15ClO3
SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)c1ccccc1Cl
Mol. weight [g/mol]: 338.78
CAS: 305374-05-4

Physical Properties

Property code	Value	Unit	Source
gf	84.64	kJ/mol	Joback Method
hf	-162.24	kJ/mol	Joback Method
hfus	37.07	kJ/mol	Joback Method
hvap	84.22	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.138		Crippen Method
mcvol	246.930	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	2833.00		NIST Webbook
tb	883.14	K	Joback Method
tc	1138.90	K	Joback Method
tf	543.77	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.15	J/mol×K	883.14	Joback Method
cpg	742.15	J/mol×K	1096.27	Joback Method
cpg	734.82	J/mol×K	1053.64	Joback Method
cpg	726.22	J/mol×K	1011.02	Joback Method
cpg	716.29	J/mol×K	968.39	Joback Method
cpg	704.95	J/mol×K	925.77	Joback Method
cpg	748.28	J/mol×K	1138.90	Joback Method

dvisc	0.0000529	Pa×s	883.14	Joback Method
dvisc	0.0000660	Pa×s	826.58	Joback Method
dvisc	0.0000850	Pa×s	770.02	Joback Method
dvisc	0.0001141	Pa×s	713.46	Joback Method
dvisc	0.0001610	Pa×s	656.89	Joback Method
dvisc	0.0002423	Pa×s	600.33	Joback Method
dvisc	0.0003973	Pa×s	543.77	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=C305374054&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