

3-Chlorobenzoic acid, 4-benzyloxyphenyl ester

Inchi:	InChI=1S/C20H15ClO3/c21-17-8-4-7-16(13-17)20(22)24-19-11-9-18(10-12-19)23-14-15-
InchiKey:	OXDQIRUYOFHTSN-UHFFFAOYSA-N
Formula:	C20H15ClO3
SMILES:	O=C(Oc1ccc(OCc2ccccc2)cc1)c1cccc(Cl)c1
Mol. weight [g/mol]:	338.78

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
rinpola	2970.00		NIST Webbook
tb	883.14	K	Joback Method
tc	1138.90	K	Joback Method
tf	543.77	K	Joback Method
vc	0.922	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.15	J/molxK	883.14	Joback Method
cpg	704.95	J/molxK	925.77	Joback Method
cpg	716.29	J/molxK	968.39	Joback Method
cpg	726.22	J/molxK	1011.02	Joback Method
cpg	734.82	J/molxK	1053.64	Joback Method
cpg	742.15	J/molxK	1096.27	Joback Method
cpg	748.28	J/molxK	1138.90	Joback Method
dvisc	0.0003973	Paxs	543.77	Joback Method
dvisc	0.0002423	Paxs	600.33	Joback Method

dvisc	0.0001610	Paxs	656.89	Joback Method
dvisc	0.0001141	Paxs	713.46	Joback Method
dvisc	0.0000850	Paxs	770.02	Joback Method
dvisc	0.0000660	Paxs	826.58	Joback Method
dvisc	0.0000529	Paxs	883.14	Joback Method

Sources

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=U357792&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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

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