3-Chloro-2-fluorobenzoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C20H14ClFO3/c21-18-8-4-7-17(19(18)22)20(23)25-16-11-9-15(10-12-16)24-13

InchiKey: BXWPFPGCSCFRHW-UHFFFAOYSA-N

Formula: C20H14ClFO3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)c1cccc(Cl)c1F

Mol. weight [g/mol]: 356.77

Physical Properties

Property code	Value	Unit	Source
gf	-119.80	kJ/mol	Joback Method
hf	-369.82	kJ/mol	Joback Method
hfus	39.76	kJ/mol	Joback Method
hvap	84.06	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.277		Crippen Method
mcvol	248.700	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	2969.00		NIST Webbook
rinpol	2969.00		NIST Webbook
tb	887.39	K	Joback Method
tc	1134.57	K	Joback Method
tf	556.88	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.95	J/mol×K	887.39	Joback Method
cpg	710.06	J/mol×K	928.59	Joback Method
cpg	720.79	J/mol×K	969.78	Joback Method
cpg	730.19	J/mol×K	1010.98	Joback Method
cpg	738.32	J/mol×K	1052.18	Joback Method
cpg	745.24	J/mol×K	1093.38	Joback Method
cpg	750.98	J/mol×K	1134.57	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=U357735&Units=SI

Legend

cpg:	Ideal gas heat capacity
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