3-Fluorobenzoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C20H15FO3/c21-17-8-4-7-16(13-17)20(22)24-19-11-9-18(10-12-19)23-14-15-5
InchiKey: VITWHNCNPZBBSV-UHFFFAOYSA-N
Formula: C20H15FO3
SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)c1cccc(F)c1
Mol. weight [g/mol]: 322.33

Physical Properties

Property code	Value	Unit	Source
gf	-98.24	kJ/mol	Joback Method
hf	-342.61	kJ/mol	Joback Method
hfus	35.96	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	4.624		Crippen Method
mcvol	236.460	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook
tb	844.98	K	Joback Method
tc	1089.34	K	Joback Method
tf	514.44	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.62	J/mol×K	844.98	Joback Method
cpg	691.37	J/mol×K	885.71	Joback Method
cpg	703.70	J/mol×K	926.43	Joback Method
cpg	714.68	J/mol×K	967.16	Joback Method
cpg	724.36	J/mol×K	1007.89	Joback Method
cpg	732.79	J/mol×K	1048.62	Joback Method
cpg	740.04	J/mol×K	1089.34	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=U307732&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