2,6-Difluorobenzoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C20H14F2O3/c21-17-7-4-8-18(22)19(17)20(23)25-16-11-9-15(10-12-16)24-13-

InchiKey: GUTALXCQRAGJFX-UHFFFAOYSA-N

Formula: C20H14F2O3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)c1c(F)cccc1F

Mol. weight [g/mol]: 340.32

Physical Properties

Property code	Value	Unit	Source
gf	-302.68	kJ/mol	Joback Method
hf	-550.19	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	78.86	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	4.763		Crippen Method
mcvol	238.230	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	2568.00		NIST Webbook
tb	849.23	K	Joback Method
tc	1085.47	K	Joback Method
tf	527.55	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.71	J/mol×K	849.23	Joback Method
cpg	696.74	J/mol×K	888.60	Joback Method
cpg	708.45	J/mol×K	927.98	Joback Method
cpg	718.89	J/mol×K	967.35	Joback Method
cpg	728.10	J/mol×K	1006.73	Joback Method
cpg	736.12	J/mol×K	1046.10	Joback Method
cpg	742.99	J/mol×K	1085.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307564&Units=SI
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

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