3,4-Difluorobenzoic acid, 2-(1-phenyleth-1-yl)-4-methoxyphenyl ester

Inchi: InChI=1S/C22H18F2O3/c1-14(15-6-4-3-5-7-15)18-13-17(26-2)9-11-21(18)27-22(25)16-8

InchiKey: VLBBGPHBSAAOFB-UHFFFAOYSA-N

Formula: C22H18F2O3

SMILES: COc1ccc(OC(=O)c2ccc(F)c(F)c2)c(C(C)c2ccccc2)c1

Mol. weight [g/mol]: 368.37

Physical Properties

Property code	Value	Unit	Source
gf	-297.91	kJ/mol	Joback Method
hf	-608.22	kJ/mol	Joback Method
hfus	39.91	kJ/mol	Joback Method
hvap	83.59	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.344		Crippen Method
mcvol	266.410	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	2584.00		NIST Webbook
rinpol	2584.00		NIST Webbook
tb	899.53	K	Joback Method
tc	1134.12	K	Joback Method
tf	547.61	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.11	J/mol×K	899.53	Joback Method
cpg	809.33	J/mol×K	938.63	Joback Method
cpg	821.16	J/mol×K	977.73	Joback Method
cpg	831.63	J/mol×K	1016.83	Joback Method
cpg	840.79	J/mol×K	1055.92	Joback Method
cpg	848.69	J/mol×K	1095.02	Joback Method
cpg	855.35	J/mol×K	1134.12	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=U358129&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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