2,6-Difluoro-3-methylbenzoic acid, 2-(1-phenyleth-1-yl)-4-methoxyphenyl ester

Inchi: InChI=1S/C23H20F2O3/c1-14-9-11-19(24)21(22(14)25)23(26)28-20-12-10-17(27-3)13-18

InchiKey: WJZWYIRKEJRNNN-UHFFFAOYSA-N

Formula: C23H20F2O3

SMILES: COc1ccc(OC(=O)c2c(F)ccc(C)c2F)c(C(C)c2ccccc2)c1

Mol. weight [g/mol]: 382.40

Physical Properties

Property code	Value	Unit	Source
gf	-299.12	kJ/mol	Joback Method
hf	-640.33	kJ/mol	Joback Method
hfus	42.12	kJ/mol	Joback Method
hvap	86.47	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	5.653		Crippen Method
mcvol	280.500	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
rinpol	2764.00		NIST Webbook
tb	927.39	K	Joback Method
tc	1160.75	K	Joback Method
tf	571.40	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.51	J/mol×K	927.39	Joback Method
cpg	865.63	J/mol×K	966.28	Joback Method
cpg	877.31	J/mol×K	1005.18	Joback Method
cpg	887.61	J/mol×K	1044.07	Joback Method
cpg	896.56	J/mol×K	1082.96	Joback Method
cpg	904.18	J/mol×K	1121.86	Joback Method
cpg	910.53	J/mol×K	1160.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358109&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