2,4,5-Trifluoro-3-methoxybenzoic acid, 2-(1-phenyleth-1-yl)-4-methoxyphenyl ester

Inchi: InChI=1S/C23H19F3O4/c1-13(14-7-5-4-6-8-14)16-11-15(28-2)9-10-19(16)30-23(27)17-1

InchiKey: QVGKRNVGTXBFBH-UHFFFAOYSA-N

Formula: C23H19F3O4

SMILES: COc1ccc(OC(=O)c2cc(F)c(F)c(OC)c2F)c(C(C)c2ccccc2)c1

Mol. weight [g/mol]: 416.39

Physical Properties

Property code	Value	Unit	Source
gf	-608.56	kJ/mol	Joback Method
hf	-980.13	kJ/mol	Joback Method
hfus	45.99	kJ/mol	Joback Method
hvap	88.73	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	5.492		Crippen Method
mcvol	288.140	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	2759.00		NIST Webbook
tb	954.06	K	Joback Method
tc	1182.40	K	Joback Method
tf	606.74	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.52	J/mol×K	954.06	Joback Method
cpg	896.15	J/mol×K	992.12	Joback Method
cpg	906.26	J/mol×K	1030.17	Joback Method
cpg	914.87	J/mol×K	1068.23	Joback Method
cpg	921.99	J/mol×K	1106.28	Joback Method
cpg	927.62	J/mol×K	1144.34	Joback Method
cpg	931.78	J/mol×K	1182.40	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=U358073&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