3-Fluoro-6-trifluoromethylbenzoic acid, 2-(1-phenyleth-1-yl)-4-methoxyphenyl ester

Inchi: InChI=1S/C23H18F4O3/c1-14(15-6-4-3-5-7-15)18-13-17(29-2)9-11-21(18)30-22(28)19-1

InchiKey: DKBWHCRDNDVQRC-UHFFFAOYSA-N

Formula: C23H18F4O3

SMILES: COc1ccc(OC(=O)c2cc(F)ccc2C(F)(F)F)c(C(C)c2ccccc2)c1

Mol. weight [g/mol]: 418.38

Physical Properties

Property code	Value	Unit	Source
gf	-676.27	kJ/mol	Joback Method
hf	-1029.83	kJ/mol	Joback Method
hfus	41.25	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	6.224		Crippen Method
mcvol	284.040	ml/mol	McGowan Method
pc	1460.13	kPa	Joback Method
rinpol	2515.00		NIST Webbook
rinpol	2515.00		NIST Webbook
tb	917.72	K	Joback Method
tc	1145.42	K	Joback Method
tf	562.48	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.82	J/mol×K	917.72	Joback Method
cpg	881.40	J/mol×K	955.67	Joback Method
cpg	892.71	J/mol×K	993.62	Joback Method
cpg	902.83	J/mol×K	1031.57	Joback Method
cpg	911.83	J/mol×K	1069.52	Joback Method
cpg	919.78	J/mol×K	1107.47	Joback Method
cpg	926.76	J/mol×K	1145.42	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=U358085&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