

3-Fluoro-5-trifluoromethylbenzoic acid, 2-(1-phenyleth-1-yl)-4-methoxyphenyl ester

Inchi:	InChI=1S/C23H18F4O3/c1-14(15-6-4-3-5-7-15)20-13-19(29-2)8-9-21(20)30-22(28)16-10
InchiKey:	VFJUCAA VZAWOGR-UHFFFAOYSA-N
Formula:	C23H18F4O3
SMILES:	COc1ccc(OC(=O)c2cc(F)cc(C(F)(F)F)c2)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	2431.00		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/molxK	917.72	Joback Method
cpg	881.40	J/molxK	955.67	Joback Method
cpg	892.71	J/molxK	993.62	Joback Method
cpg	902.83	J/molxK	1031.57	Joback Method
cpg	911.83	J/molxK	1069.52	Joback Method
cpg	919.78	J/molxK	1107.47	Joback Method
cpg	926.76	J/molxK	1145.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358153&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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

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