

2,4,5-Trifluoro-3-methoxybenzoic acid, phenyl ester

Inchi:	InChI=1S/C14H9F3O3/c1-19-13-11(16)9(7-10(15)12(13)17)14(18)20-8-5-3-2-4-6-8/h2-7H
InchiKey:	JLPDXBRAYFXHIQ-UHFFFAOYSA-N
Formula:	C14H9F3O3
SMILES:	COc1c(F)c(F)cc(C(=O)Oc2ccccc2)c1F
Mol. weight [g/mol]:	282.21

Physical Properties

Property code	Value	Unit	Source
gf	-670.05	kJ/mol	Joback Method
hf	-870.46	kJ/mol	Joback Method
hfus	31.76	kJ/mol	Joback Method
hvap	63.07	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.332		Crippen Method
mcvol	179.220	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	1841.00		NIST Webbook
tb	689.52	K	Joback Method
tc	901.81	K	Joback Method
tf	446.62	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.63	J/mol×K	689.52	Joback Method
cpg	472.83	J/mol×K	724.90	Joback Method
cpg	484.20	J/mol×K	760.28	Joback Method
cpg	494.75	J/mol×K	795.67	Joback Method
cpg	504.48	J/mol×K	831.05	Joback Method
cpg	513.39	J/mol×K	866.43	Joback Method
cpg	521.47	J/mol×K	901.81	Joback Method

Sources

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=U357611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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