2,4,5-Trifluoro-3-methoxybenzamide, N-(4-fluorophenyl)-

Inchi: InChI=1S/C14H9F4NO2/c1-21-13-11(17)9(6-10(16)12(13)18)14(20)19-8-4-2-7(15)3-5-8/h
InchiKey: ROMCVTXEZNFZIV-UHFFFAOYSA-N
Formula: C14H9F4NO2
SMILES: COc1c(F)c(F)cc(C(=O)Nc2ccc(F)cc2)c1F
Mol. weight [g/mol]: 299.22

Physical Properties

Property code	Value	Unit	Source
gf	-680.10	kJ/mol	Joback Method
hf	-892.35	kJ/mol	Joback Method
hfus	38.36	kJ/mol	Joback Method
hvap	66.94	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.504		Crippen Method
mcvol	185.100	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	2072.00		NIST Webbook
tb	721.52	K	Joback Method
tc	928.16	K	Joback Method
tf	490.16	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.10	J/mol×K	721.52	Joback Method
cpg	503.47	J/mol×K	755.96	Joback Method
cpg	514.04	J/mol×K	790.40	Joback Method
cpg	523.83	J/mol×K	824.84	Joback Method
cpg	532.86	J/mol×K	859.28	Joback Method
cpg	541.14	J/mol×K	893.72	Joback Method
cpg	548.67	J/mol×K	928.16	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=U358065&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