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

Inchi: InChI=1S/C14H8F3NO5/c1-22-13-11(16)9(6-10(15)12(13)17)14(19)23-8-4-2-7(3-5-8)18(

InchiKey: XJTAUUAMKKAXOJ-UHFFFAOYSA-N

Formula: C14H8F3NO5

SMILES: COc1c(F)c(F)cc(C(=O)Oc2ccc([N+](=O)[O-])cc2)c1F

Mol. weight [g/mol]: 327.21

Physical Properties

Property code	Value	Unit	Source
gf	-644.13	kJ/mol	Joback Method
hf	-892.69	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	80.33	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	3.240		Crippen Method
mcvol	196.640	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	846.34	K	Joback Method
tc	1078.32	K	Joback Method
tf	602.75	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.73	J/mol×K	846.34	Joback Method
cpg	560.37	J/mol×K	885.00	Joback Method
cpg	568.95	J/mol×K	923.67	Joback Method
cpg	576.48	J/mol×K	962.33	Joback Method
cpg	582.96	J/mol×K	1000.99	Joback Method
cpg	588.39	J/mol×K	1039.65	Joback Method
cpg	592.76	J/mol×K	1078.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U357620&Units=SI

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