3-Methoxy-2,4,5-trifluorobenzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C14H4F8O3/c1-24-12-5(16)3(2-4(15)6(12)17)14(23)25-13-10(21)8(19)7(18)9(2

InchiKey: CBCCZOBRSVJIKZ-UHFFFAOYSA-N

Formula: C14H4F8O3

SMILES: COc1c(F)c(F)cc(C(=O)Oc2c(F)c(F)c(F)c(F)c2F)c1F

Mol. weight [g/mol]: 372.17

Physical Properties

Property code	Value	Unit	Source
gf	-1692.25	kJ/mol	Joback Method
hf	-1908.36	kJ/mol	Joback Method
hfus	45.21	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	4.027		Crippen Method
mcvol	188.070	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook
tb	710.77	K	Joback Method
tc	892.37	K	Joback Method
tf	512.17	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.75	J/mol×K	710.77	Joback Method
cpg	503.10	J/mol×K	741.04	Joback Method
cpg	511.92	J/mol×K	771.30	Joback Method
cpg	520.19	J/mol×K	801.57	Joback Method
cpg	527.90	J/mol×K	831.83	Joback Method
cpg	535.03	J/mol×K	862.10	Joback Method
cpg	541.57	J/mol×K	892.37	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=U360570&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

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