3-Methoxybenzoic acid, 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C16H11F5O4/c1-23-9-4-2-3-8(7-9)16(22)25-6-5-24-15-13(20)11(18)10(17)12(1

InchiKey: YOFMJAQVPLXERA-UHFFFAOYSA-N

Formula: C16H11F5O4

SMILES: COc1cccc(C(=O)OCCOc2c(F)c(F)c(F)c(F)c2F)c1

Mol. weight [g/mol]: 362.25

Physical Properties

Property code	Value	Unit	Source
gf	-1167.09	kJ/mol	Joback Method
hf	-1459.12	kJ/mol	Joback Method
hfus	43.51	kJ/mol	Joback Method
hvap	69.62	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	3.626		Crippen Method
mcvol	216.810	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	766.20	K	Joback Method
tc	960.94	K	Joback Method
tf	517.61	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.99	J/mol×K	766.20	Joback Method
cpg	615.70	J/mol×K	798.66	Joback Method
cpg	626.58	J/mol×K	831.11	Joback Method
cpg	636.62	J/mol×K	863.57	Joback Method
cpg	645.81	J/mol×K	896.03	Joback Method
cpg	654.14	J/mol×K	928.48	Joback Method
cpg	661.58	J/mol×K	960.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374933&Units=SI
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

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