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

Inchi: InChI=1S/C13H7F11O3/c1-26-8-6(15)4(2-5(14)7(8)16)9(25)27-3-11(19,20)13(23,24)12(2

InchiKey: PKWXUXRRKWCQNO-UHFFFAOYSA-N

Formula: C13H7F11O3

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

Mol. weight [g/mol]: 420.18

Physical Properties

Property code	Value	Unit	Source
gf	-2343.28	kJ/mol	Joback Method
hf	-2686.76	kJ/mol	Joback Method
hfus	34.00	kJ/mol	Joback Method
hvap	47.76	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.440		Crippen Method
mcvol	203.050	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	1455.00		NIST Webbook
tb	623.99	K	Joback Method
tc	782.61	K	Joback Method
tf	405.91	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.73	J/mol×K	623.99	Joback Method
cpg	577.43	J/mol×K	650.43	Joback Method
cpg	587.49	J/mol×K	676.86	Joback Method
cpg	596.93	J/mol×K	703.30	Joback Method
cpg	605.78	J/mol×K	729.74	Joback Method
cpg	614.06	J/mol×K	756.17	Joback Method
cpg	621.79	J/mol×K	782.61	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=U360567&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