Methyl 2-hydroxy-4-methoxybenzoate, heptafluorobutyrate

Inchi: InChI=1S/C13H9F7O5/c1-23-6-3-4-7(9(21)24-2)8(5-6)25-10(22)11(14,15)12(16,17)13(18

InchiKey: JWQLCRJNNHRNSJ-UHFFFAOYSA-N

Formula: C13H9F7O5

SMILES: COC(=O)c1ccc(OC)cc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 378.20

Physical Properties

Property code	Value	Unit	Source
gf	-1776.26	kJ/mol	Joback Method
hf	-2118.90	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	59.25	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.220		Crippen Method
mcvol	203.410	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1521.00		NIST Webbook
rinpol	1521.00		NIST Webbook
tb	693.68	K	Joback Method
tc	877.67	K	Joback Method
tf	465.67	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.61	J/mol×K	693.68	Joback Method
cpg	587.43	J/mol×K	724.34	Joback Method
cpg	597.45	J/mol×K	755.01	Joback Method
cpg	606.70	J/mol×K	785.67	Joback Method
cpg	615.23	J/mol×K	816.34	Joback Method
cpg	623.06	J/mol×K	847.00	Joback Method
cpg	630.22	J/mol×K	877.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375950&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

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