Methyl 2-hydroxy-4-methoxybenzoate, trifluoroacetate

Inchi: InChI=1S/C11H9F3O5/c1-17-6-3-4-7(9(15)18-2)8(5-6)19-10(16)11(12,13)14/h3-5H,1-2H

InchiKey: LUMDSUIKDRGIEW-UHFFFAOYSA-N

Formula: C11H9F3O5

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

Mol. weight [g/mol]: 278.18

Physical Properties

Property code	Value	Unit	Source
gf	-1019.54	kJ/mol	Joback Method
hf	-1275.68	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	60.66	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.950		Crippen Method
mcvol	168.150	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1482.00		NIST Webbook
rinpol	1482.00		NIST Webbook
tb	657.30	K	Joback Method
tc	855.60	K	Joback Method
tf	435.93	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.65	J/mol×K	657.30	Joback Method
cpg	448.70	J/mol×K	690.35	Joback Method
cpg	459.06	J/mol×K	723.40	Joback Method
cpg	468.71	J/mol×K	756.45	Joback Method
cpg	477.68	J/mol×K	789.50	Joback Method
cpg	485.94	J/mol×K	822.55	Joback Method
cpg	493.51	J/mol×K	855.60	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=U375951&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