Methyl salicylate, Gly, TFA

Inchi: InChI=1S/C22H14F12O12/c1-40-13(35)7-4-2-3-5-8(7)42-14-12(46-18(39)22(32,33)34)11
InchiKey: NWJNOOFMDOXMLR-HNRZYHPDSA-N
Formula: C22H14F12O12
SMILES: COC(=O)c1ccccc1OC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1
Mol. weight [g/mol]: 698.32

Physical Properties

Property code	Value	Unit	Source
gf	-3456.33	kJ/mol	Joback Method
hf	-4175.93	kJ/mol	Joback Method
hfus	72.91	kJ/mol	Joback Method
hvap	104.41	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	3.105		Crippen Method
mcvol	356.400	ml/mol	McGowan Method
pc	975.95	kPa	Joback Method
rinpol	1970.00		NIST Webbook
rinpol	1963.00		NIST Webbook
tb	1144.43	K	Joback Method
tc	1432.36	K	Joback Method
tf	793.42	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.27	J/mol×K	1144.43	Joback Method
cpg	1230.21	J/mol×K	1192.42	Joback Method
cpg	1227.04	J/mol×K	1240.41	Joback Method
cpg	1220.82	J/mol×K	1288.39	Joback Method
cpg	1211.64	J/mol×K	1336.38	Joback Method
cpg	1199.58	J/mol×K	1384.37	Joback Method
cpg	1184.71	J/mol×K	1432.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R394742&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