o-Hydroxyphenylacetic acid, TFA-ME

Inchi: InChI=1S/C11H9F3O4/c1-17-9(15)6-7-4-2-3-5-8(7)18-10(16)11(12,13)14/h2-5H,6H2,1H3
InchiKey: UXGADNRIZFNNOW-UHFFFAOYSA-N
Formula: C11H9F3O4
SMILES: COC(=O)Cc1ccccc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 262.18

Physical Properties

Property code	Value	Unit	Source
gf	-904.91	kJ/mol	Joback Method
hf	-1131.99	kJ/mol	Joback Method
hfus	25.30	kJ/mol	Joback Method
hvap	57.58	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.870		Crippen Method
mcvol	162.280	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1245.00		NIST Webbook
rinpol	1245.00		NIST Webbook
tb	629.90	K	Joback Method
tc	828.90	K	Joback Method
tf	401.18	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.71	J/mol×K	629.90	Joback Method
cpg	426.13	J/mol×K	663.07	Joback Method
cpg	436.81	J/mol×K	696.23	Joback Method
cpg	446.75	J/mol×K	729.40	Joback Method
cpg	455.99	J/mol×K	762.57	Joback Method
cpg	464.53	J/mol×K	795.73	Joback Method
cpg	472.40	J/mol×K	828.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R387249&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