Vanillylmandelic acid, TFA-ME

Inchi: InChI=1S/C14H10F6O7/c1-24-8-5-6(3-4-7(8)26-11(22)13(15,16)17)9(10(21)25-2)27-12(2
InchiKey: LDMNEDDQGWVLPK-UHFFFAOYSA-N
Formula: C14H10F6O7
SMILES: COC(=O)C(OC(=O)C(F)(F)F)c1ccc(OC(=O)C(F)(F)F)c(OC)c1
Mol. weight [g/mol]: 404.22

Physical Properties

Property code	Value	Unit	Source
gf	-1812.23	kJ/mol	Joback Method
hf	-2184.76	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	72.35	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.482		Crippen Method
mcvol	223.170	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	1440.00		NIST Webbook
rinpol	1440.00		NIST Webbook
tb	796.37	K	Joback Method
tc	989.43	K	Joback Method
tf	531.09	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.01	J/mol×K	796.37	Joback Method
cpg	665.89	J/mol×K	828.55	Joback Method
cpg	674.89	J/mol×K	860.72	Joback Method
cpg	683.02	J/mol×K	892.90	Joback Method
cpg	690.28	J/mol×K	925.07	Joback Method
cpg	696.71	J/mol×K	957.25	Joback Method
cpg	702.29	J/mol×K	989.43	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=R387303&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