Vanillin, pentafluoropropionate

Inchi: InChI=1S/C11H7F5O4/c1-19-8-4-6(5-17)2-3-7(8)20-9(18)10(12,13)11(14,15)16/h2-5H,1H
InchiKey: TWLVCWDHNWXSQR-UHFFFAOYSA-N
Formula: C11H7F5O4
SMILES: COc1cc(C=O)ccc1OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 298.16

Physical Properties

Property code	Value	Unit	Source
gf	-1271.92	kJ/mol	Joback Method
hf	-1517.43	kJ/mol	Joback Method
hfus	24.35	kJ/mol	Joback Method
hvap	55.29	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.611		Crippen Method
mcvol	165.820	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1332.00		NIST Webbook
tb	624.98	K	Joback Method
tc	814.52	K	Joback Method
tf	409.37	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.35	J/mol×K	624.98	Joback Method
cpg	444.76	J/mol×K	656.57	Joback Method
cpg	454.45	J/mol×K	688.16	Joback Method
cpg	463.45	J/mol×K	719.75	Joback Method
cpg	471.78	J/mol×K	751.34	Joback Method
cpg	479.47	J/mol×K	782.93	Joback Method
cpg	486.56	J/mol×K	814.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375937&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