Vanillin, trifluoroacetate

Inchi: InChI=1S/C10H7F3O4/c1-16-8-4-6(5-14)2-3-7(8)17-9(15)10(11,12)13/h2-5H,1H3
InchiKey: CZRDEKBEQVBOMB-UHFFFAOYSA-N
Formula: C10H7F3O4
SMILES: COc1cc(C=O)ccc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 248.16

Physical Properties

Property code	Value	Unit	Source
gf	-893.56	kJ/mol	Joback Method
hf	-1095.82	kJ/mol	Joback Method
hfus	23.01	kJ/mol	Joback Method
hvap	55.99	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.975		Crippen Method
mcvol	148.190	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpol	1314.00		NIST Webbook
rinpol	1314.00		NIST Webbook
tb	606.79	K	Joback Method
tc	805.18	K	Joback Method
tf	394.50	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.06	J/mol×K	606.79	Joback Method
cpg	377.32	J/mol×K	639.86	Joback Method
cpg	386.94	J/mol×K	672.92	Joback Method
cpg	395.93	J/mol×K	705.99	Joback Method
cpg	404.31	J/mol×K	739.05	Joback Method
cpg	412.08	J/mol×K	772.12	Joback Method
cpg	419.26	J/mol×K	805.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375935&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