Vanillin, heptafluorobutyrate

Inchi: InChI=1S/C12H7F7O4/c1-22-8-4-6(5-20)2-3-7(8)23-9(21)10(13,14)11(15,16)12(17,18)19
InchiKey: GJEXMEDKOQTZTK-UHFFFAOYSA-N
Formula: C12H7F7O4
SMILES: COc1cc(C=O)ccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 348.17

Physical Properties

Property code	Value	Unit	Source
gf	-1650.28	kJ/mol	Joback Method
hf	-1939.04	kJ/mol	Joback Method
hfus	25.68	kJ/mol	Joback Method
hvap	54.58	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.246		Crippen Method
mcvol	183.450	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1376.00		NIST Webbook
rinpol	1376.00		NIST Webbook
tb	643.17	K	Joback Method
tc	825.29	K	Joback Method
tf	424.24	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.57	J/mol×K	643.17	Joback Method
cpg	513.00	J/mol×K	673.52	Joback Method
cpg	522.65	J/mol×K	703.88	Joback Method
cpg	531.57	J/mol×K	734.23	Joback Method
cpg	539.80	J/mol×K	764.58	Joback Method
cpg	547.37	J/mol×K	794.94	Joback Method
cpg	554.33	J/mol×K	825.29	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=U375936&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