2,6-Dimethoxyphenol,heptafluorobutyrate

Inchi: InChI=1S/C12H9F7O4/c1-21-6-4-3-5-7(22-2)8(6)23-9(20)10(13,14)11(15,16)12(17,18)19
InchiKey: HOUIQBCSIBUBBK-UHFFFAOYSA-N
Formula: C12H9F7O4
SMILES: COc1cccc(OC)c1OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 350.19

Physical Properties

Property code	Value	Unit	Source
gf	-1655.76	kJ/mol	Joback Method
hf	-1985.68	kJ/mol	Joback Method
hfus	24.58	kJ/mol	Joback Method
hvap	50.28	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.442		Crippen Method
mcvol	187.750	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook
tb	616.93	K	Joback Method
tc	794.43	K	Joback Method
tf	404.47	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.95	J/mol×K	616.93	Joback Method
cpg	522.72	J/mol×K	646.51	Joback Method
cpg	533.72	J/mol×K	676.10	Joback Method
cpg	543.98	J/mol×K	705.68	Joback Method
cpg	553.54	J/mol×K	735.27	Joback Method
cpg	562.41	J/mol×K	764.85	Joback Method
cpg	570.63	J/mol×K	794.43	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=U374280&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