Heptafluorobutyric acid, 2-isopropoxyphenyl ester

Inchi: InChI=1S/C13H11F7O3/c1-7(2)22-8-5-3-4-6-9(8)23-10(21)11(14,15)12(16,17)13(18,19)2

InchiKey: ROJCOPNQPRDSSD-UHFFFAOYSA-N

Formula: C13H11F7O3

SMILES: CC(C)Oc1ccccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 348.21

Physical Properties

Property code	Value	Unit	Source
gf	-1535.15	kJ/mol	Joback Method
hf	-1867.91	kJ/mol	Joback Method
hfus	22.85	kJ/mol	Joback Method
hvap	49.04	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.212		Crippen Method
mcvol	195.970	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook
tb	611.97	K	Joback Method
tc	790.74	K	Joback Method
tf	365.99	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.98	J/mol×K	611.97	Joback Method
cpg	549.02	J/mol×K	641.77	Joback Method
cpg	561.17	J/mol×K	671.56	Joback Method
cpg	572.48	J/mol×K	701.36	Joback Method
cpg	582.98	J/mol×K	731.15	Joback Method
cpg	592.73	J/mol×K	760.95	Joback Method
cpg	601.77	J/mol×K	790.74	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299084&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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