2-Fluorobenzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C13H4F6O2/c14-6-4-2-1-3-5(6)13(20)21-12-10(18)8(16)7(15)9(17)11(12)19/h1
InchiKey: IHTAXFVWOYSVBK-UHFFFAOYSA-N
Formula: C13H4F6O2
SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1ccccc1F
Mol. weight [g/mol]: 306.16

Physical Properties

Property code	Value	Unit	Source
gf	-1177.16	kJ/mol	Joback Method
hf	-1328.87	kJ/mol	Joback Method
hfus	36.44	kJ/mol	Joback Method
hvap	57.31	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	3.740		Crippen Method
mcvol	164.570	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1529.00		NIST Webbook
tb	651.99	K	Joback Method
tc	845.58	K	Joback Method
tf	439.93	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.58	J/mol×K	651.99	Joback Method
cpg	418.46	J/mol×K	684.26	Joback Method
cpg	427.76	J/mol×K	716.52	Joback Method
cpg	436.47	J/mol×K	748.79	Joback Method
cpg	444.60	J/mol×K	781.05	Joback Method
cpg	452.15	J/mol×K	813.32	Joback Method
cpg	459.13	J/mol×K	845.58	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=U354701&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

Latest version available from:
https://www.chemeo.com/cid/59-780-1/2-Fluorobenzoic-acid-pentafluorophenyl-ester.pdf
Generated by Cheméo on 2024-04-29 04:12:36.257662996 +0000 UTC m=+16653205.178240311.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.