3-Fluoro-4-trifluoromethylbenzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C14H3F9O2/c15-6-3-4(1-2-5(6)14(21,22)23)13(24)25-12-10(19)8(17)7(16)9(18

InchiKey: SRLYDDSPYWLWSL-UHFFFAOYSA-N

Formula: C14H3F9O2

SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 374.16

Physical Properties

Property code	Value	Unit	Source
gf	-1759.96	kJ/mol	Joback Method
hf	-1958.06	kJ/mol	Joback Method
hfus	40.47	kJ/mol	Joback Method
hvap	56.45	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	4.759		Crippen Method
mcvol	183.970	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	1451.00		NIST Webbook
rinpol	1451.00		NIST Webbook
tb	674.43	K	Joback Method
tc	855.17	K	Joback Method
tf	467.91	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.81	J/mol×K	674.43	Joback Method
cpg	493.20	J/mol×K	704.55	Joback Method
cpg	501.99	J/mol×K	734.68	Joback Method
cpg	510.19	J/mol×K	764.80	Joback Method
cpg	517.83	J/mol×K	794.92	Joback Method
cpg	524.91	J/mol×K	825.05	Joback Method
cpg	531.46	J/mol×K	855.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360594&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