3-Fluoro-4-trifluoromethylbenzoic acid, neopentyl ester

Inchi: InChI=1S/C13H14F4O2/c1-12(2,3)7-19-11(18)8-4-5-9(10(14)6-8)13(15,16)17/h4-6H,7H2

InchiKey: VHOIKURXUZEQKN-UHFFFAOYSA-N

Formula: C13H14F4O2

SMILES: CC(C)(C)COC(=O)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 278.24

Physical Properties

Property code	Value	Unit	Source
gf	-855.75	kJ/mol	Joback Method
hf	-1144.80	kJ/mol	Joback Method
hfus	22.97	kJ/mol	Joback Method
hvap	51.43	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.047		Crippen Method
mcvol	184.790	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	1298.00		NIST Webbook
tb	600.39	K	Joback Method
tc	791.41	K	Joback Method
tf	367.09	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.60	J/mol×K	600.39	Joback Method
cpg	495.65	J/mol×K	632.23	Joback Method
cpg	508.79	J/mol×K	664.06	Joback Method
cpg	521.09	J/mol×K	695.90	Joback Method
cpg	532.59	J/mol×K	727.74	Joback Method
cpg	543.32	J/mol×K	759.58	Joback Method
cpg	553.33	J/mol×K	791.41	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=U357933&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