2-Fluoro-3-trifluoromethylbenzoic acid, hexyl ester

Inchi: InChI=1S/C14H16F4O2/c1-2-3-4-5-9-20-13(19)10-7-6-8-11(12(10)15)14(16,17)18/h6-8H

InchiKey: BDKZAQSXTXMWNU-UHFFFAOYSA-N

Formula: C14H16F4O2

SMILES: CCCCCCOC(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 292.27

Physical Properties

Property code	Value	Unit	Source
gf	-850.17	kJ/mol	Joback Method
hf	-1156.69	kJ/mol	Joback Method
hfus	32.97	kJ/mol	Joback Method
hvap	54.95	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.582		Crippen Method
mcvol	198.880	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
tb	626.50	K	Joback Method
tc	806.72	K	Joback Method
tf	375.94	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.75	J/mol×K	626.50	Joback Method
cpg	542.70	J/mol×K	656.54	Joback Method
cpg	555.89	J/mol×K	686.57	Joback Method
cpg	568.33	J/mol×K	716.61	Joback Method
cpg	580.06	J/mol×K	746.64	Joback Method
cpg	591.11	J/mol×K	776.68	Joback Method
cpg	601.49	J/mol×K	806.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338721&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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