6-Fluoro-2-trifluoromethylbenzoic acid, pentyl ester

Inchi: InChI=1S/C13H14F4O2/c1-2-3-4-8-19-12(18)11-9(13(15,16)17)6-5-7-10(11)14/h5-7H,2-4

InchiKey: OZIYMNLXXPLILM-UHFFFAOYSA-N

Formula: C13H14F4O2

SMILES: CCCCCOC(=O)c1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 278.24

Physical Properties

Property code	Value	Unit	Source
gf	-858.59	kJ/mol	Joback Method
hf	-1136.05	kJ/mol	Joback Method
hfus	30.38	kJ/mol	Joback Method
hvap	52.72	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.192		Crippen Method
mcvol	184.790	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
tb	603.62	K	Joback Method
tc	785.28	K	Joback Method
tf	364.67	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.37	J/mol×K	603.62	Joback Method
cpg	491.78	J/mol×K	633.90	Joback Method
cpg	504.45	J/mol×K	664.17	Joback Method
cpg	516.41	J/mol×K	694.45	Joback Method
cpg	527.67	J/mol×K	724.73	Joback Method
cpg	538.27	J/mol×K	755.00	Joback Method
cpg	548.24	J/mol×K	785.28	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=U338978&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