3-Fluoro-4-trifluoromethylbenzoic acid, 2-propylphenyl ester

Inchi: InChI=1S/C17H14F4O2/c1-2-5-11-6-3-4-7-15(11)23-16(22)12-8-9-13(14(18)10-12)17(19

InchiKey: VMRCDXTZDZZKLQ-UHFFFAOYSA-N

Formula: C17H14F4O2

SMILES: CCCc1ccccc1OC(=O)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 326.29

Physical Properties

Property code	Value	Unit	Source
gf	-722.13	kJ/mol	Joback Method
hf	-993.55	kJ/mol	Joback Method
hfus	34.39	kJ/mol	Joback Method
hvap	64.57	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.016		Crippen Method
mcvol	217.390	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1811.00		NIST Webbook
tb	726.80	K	Joback Method
tc	933.63	K	Joback Method
tf	448.69	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.27	J/mol×K	726.80	Joback Method
cpg	617.00	J/mol×K	761.27	Joback Method
cpg	629.74	J/mol×K	795.74	Joback Method
cpg	641.53	J/mol×K	830.21	Joback Method
cpg	652.43	J/mol×K	864.69	Joback Method
cpg	662.48	J/mol×K	899.16	Joback Method
cpg	671.73	J/mol×K	933.63	Joback Method

Sources

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=U360598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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