2-Fluorobenzoic acid, 2-propylphenyl ester

Inchi: InChI=1S/C16H15FO2/c1-2-7-12-8-3-6-11-15(12)19-16(18)13-9-4-5-10-14(13)17/h3-6,8-
InchiKey: WGVQROIYXXIALG-UHFFFAOYSA-N
Formula: C16H15FO2
SMILES: CCCc1ccccc1OC(=O)c1ccccc1F
Mol. weight [g/mol]: 258.29

Physical Properties

Property code	Value	Unit	Source
gf	-139.33	kJ/mol	Joback Method
hf	-364.36	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	65.42	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	3.997		Crippen Method
mcvol	197.990	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1938.00		NIST Webbook
rinpol	1938.00		NIST Webbook
tb	704.36	K	Joback Method
tc	928.88	K	Joback Method
tf	420.71	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.95	J/mol×K	704.36	Joback Method
cpg	540.01	J/mol×K	741.78	Joback Method
cpg	553.98	J/mol×K	779.20	Joback Method
cpg	566.90	J/mol×K	816.62	Joback Method
cpg	578.80	J/mol×K	854.04	Joback Method
cpg	589.72	J/mol×K	891.46	Joback Method
cpg	599.71	J/mol×K	928.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354704&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