2,4-Difluorobenzoic acid, 2-propylphenyl ester

Inchi: InChI=1S/C16H14F2O2/c1-2-5-11-6-3-4-7-15(11)20-16(19)13-9-8-12(17)10-14(13)18/h3
InchiKey: FZOUBYMAECBBBL-UHFFFAOYSA-N
Formula: C16H14F2O2
SMILES: CCCc1ccccc1OC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 276.28

Physical Properties

Property code	Value	Unit	Source
gf	-343.77	kJ/mol	Joback Method
hf	-571.94	kJ/mol	Joback Method
hfus	33.06	kJ/mol	Joback Method
hvap	65.27	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.136		Crippen Method
mcvol	199.760	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	1846.00		NIST Webbook
rinpol	1846.00		NIST Webbook
tb	708.61	K	Joback Method
tc	924.70	K	Joback Method
tf	433.82	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.87	J/mol×K	708.61	Joback Method
cpg	546.09	J/mol×K	744.62	Joback Method
cpg	559.33	J/mol×K	780.64	Joback Method
cpg	571.60	J/mol×K	816.65	Joback Method
cpg	582.95	J/mol×K	852.67	Joback Method
cpg	593.39	J/mol×K	888.68	Joback Method
cpg	602.96	J/mol×K	924.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360559&Units=SI

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