2,6-Difluoro-3-methylbenzoic acid, isopropyl ester

Inchi: InChI=1S/C11H12F2O2/c1-6(2)15-11(14)9-8(12)5-4-7(3)10(9)13/h4-6H,1-3H3
InchiKey: ZJWYLCZNZWGVEW-UHFFFAOYSA-N
Formula: C11H12F2O2
SMILES: Cc1ccc(F)c(C(=O)OC(C)C)c1F
Mol. weight [g/mol]: 214.21

Physical Properties

Property code	Value	Unit	Source
gf	-500.72	kJ/mol	Joback Method
hf	-710.55	kJ/mol	Joback Method
hfus	22.54	kJ/mol	Joback Method
hvap	51.48	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	2.838		Crippen Method
mcvol	153.070	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
rinpol	1292.00		NIST Webbook
rinpol	1292.00		NIST Webbook
tb	567.09	K	Joback Method
tc	764.10	K	Joback Method
tf	336.05	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.24	J/mol×K	567.09	Joback Method
cpg	374.86	J/mol×K	599.92	Joback Method
cpg	386.89	J/mol×K	632.76	Joback Method
cpg	398.31	J/mol×K	665.59	Joback Method
cpg	409.14	J/mol×K	698.43	Joback Method
cpg	419.38	J/mol×K	731.26	Joback Method
cpg	429.03	J/mol×K	764.10	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=U357673&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