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

Inchi: InChI=1S/C10H10F2O2/c1-3-14-10(13)8-7(11)5-4-6(2)9(8)12/h4-5H,3H2,1-2H3
InchiKey: IWFXOLBZIKXIRR-UHFFFAOYSA-N
Formula: C10H10F2O2
SMILES: CCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 200.18

Physical Properties

Property code	Value	Unit	Source
gf	-506.70	kJ/mol	Joback Method
hf	-684.63	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	49.64	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.450		Crippen Method
mcvol	138.980	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1269.00		NIST Webbook
rinpol	1269.00		NIST Webbook
tb	544.65	K	Joback Method
tc	740.32	K	Joback Method
tf	339.78	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.13	J/mol×K	544.65	Joback Method
cpg	327.55	J/mol×K	577.26	Joback Method
cpg	338.45	J/mol×K	609.87	Joback Method
cpg	348.84	J/mol×K	642.49	Joback Method
cpg	358.71	J/mol×K	675.10	Joback Method
cpg	368.07	J/mol×K	707.71	Joback Method
cpg	376.92	J/mol×K	740.32	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=U338838&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