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

Inchi: InChI=1S/C9H8F2O2/c1-5-3-4-6(10)7(8(5)11)9(12)13-2/h3-4H,1-2H3
InchiKey: GFNPHCOGNULPLS-UHFFFAOYSA-N
Formula: C9H8F2O2
SMILES: COC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 186.16

Physical Properties

Property code	Value	Unit	Source
gf	-515.12	kJ/mol	Joback Method
hf	-663.99	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	47.41	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.060		Crippen Method
mcvol	124.890	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1212.00		NIST Webbook
tb	521.77	K	Joback Method
tc	720.11	K	Joback Method
tf	328.51	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.27	J/mol×K	521.77	Joback Method
cpg	282.66	J/mol×K	554.83	Joback Method
cpg	292.60	J/mol×K	587.88	Joback Method
cpg	302.08	J/mol×K	620.94	Joback Method
cpg	311.10	J/mol×K	653.99	Joback Method
cpg	319.66	J/mol×K	687.05	Joback Method
cpg	327.76	J/mol×K	720.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357689&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

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