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

Inchi: InChI=1S/C12H14F2O2/c1-7(2)6-16-12(15)10-9(13)5-4-8(3)11(10)14/h4-5,7H,6H2,1-3H3

InchiKey: ZFCUZWIAYRXTCL-UHFFFAOYSA-N

Formula: C12H14F2O2

SMILES: Cc1ccc(F)c(C(=O)OCC(C)C)c1F

Mol. weight [g/mol]: 228.24

Physical Properties

Property code	Value	Unit	Source
gf	-492.30	kJ/mol	Joback Method
hf	-731.19	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	53.70	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.086		Crippen Method
mcvol	167.160	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	1454.00		NIST Webbook
rinpol	1454.00		NIST Webbook
tb	589.97	K	Joback Method
tc	784.39	K	Joback Method
tf	347.32	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.75	J/mol×K	589.97	Joback Method
cpg	423.16	J/mol×K	622.37	Joback Method
cpg	435.93	J/mol×K	654.78	Joback Method
cpg	448.05	J/mol×K	687.18	Joback Method
cpg	459.52	J/mol×K	719.58	Joback Method
cpg	470.37	J/mol×K	751.99	Joback Method
cpg	480.58	J/mol×K	784.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338839&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