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

Inchi: InChI=1S/C13H16F2O2/c1-3-4-5-8-17-13(16)11-10(14)7-6-9(2)12(11)15/h6-7H,3-5,8H2,
InchiKey: APCOKOCFDKVPJD-UHFFFAOYSA-N
Formula: C13H16F2O2
SMILES: CCCCCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 242.26

Physical Properties

Property code	Value	Unit	Source
gf	-481.44	kJ/mol	Joback Method
hf	-746.55	kJ/mol	Joback Method
hfus	31.25	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.620		Crippen Method
mcvol	181.250	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1587.00		NIST Webbook
rinpol	1587.00		NIST Webbook
tb	613.29	K	Joback Method
tc	801.92	K	Joback Method
tf	373.59	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.48	J/mol×K	613.29	Joback Method
cpg	472.29	J/mol×K	644.73	Joback Method
cpg	485.43	J/mol×K	676.17	Joback Method
cpg	497.92	J/mol×K	707.61	Joback Method
cpg	509.76	J/mol×K	739.04	Joback Method
cpg	520.96	J/mol×K	770.48	Joback Method
cpg	531.52	J/mol×K	801.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338841&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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