2,4-Difluorobenzoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C13H16F2O3/c1-9(5-6-17-2)8-18-13(16)11-4-3-10(14)7-12(11)15/h3-4,7,9H,5-

InchiKey: MNPVEZYRRIXDBB-UHFFFAOYSA-N

Formula: C13H16F2O3

SMILES: COCCC(C)COC(=O)c1ccc(F)cc1F

Mol. weight [g/mol]: 258.26

Physical Properties

Property code	Value	Unit	Source
gf	-579.25	kJ/mol	Joback Method
hf	-872.58	kJ/mol	Joback Method
hfus	29.30	kJ/mol	Joback Method
hvap	57.68	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.794		Crippen Method
mcvol	187.120	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1624.00		NIST Webbook
tb	630.29	K	Joback Method
tc	820.21	K	Joback Method
tf	368.30	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.51	J/mol×K	630.29	Joback Method
cpg	499.58	J/mol×K	661.94	Joback Method
cpg	512.94	J/mol×K	693.60	Joback Method
cpg	525.60	J/mol×K	725.25	Joback Method
cpg	537.55	J/mol×K	756.90	Joback Method
cpg	548.80	J/mol×K	788.56	Joback Method
cpg	559.35	J/mol×K	820.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360558&Units=SI

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