2,4-Difluorobenzoic acid, 3-methylbutyl-2 ester

Inchi: InChI=1S/C12H14F2O2/c1-7(2)8(3)16-12(15)10-5-4-9(13)6-11(10)14/h4-8H,1-3H3
InchiKey: CHECDZKHGXJPLQ-UHFFFAOYSA-N
Formula: C12H14F2O2
SMILES: CC(C)C(C)OC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 228.24

Physical Properties

Property code	Value	Unit	Source
gf	-485.11	kJ/mol	Joback Method
hf	-725.00	kJ/mol	Joback Method
hfus	22.00	kJ/mol	Joback Method
hvap	52.65	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.166		Crippen Method
mcvol	167.160	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1354.00		NIST Webbook
tb	584.55	K	Joback Method
tc	781.81	K	Joback Method
tf	319.80	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.56	J/mol×K	584.55	Joback Method
cpg	424.52	J/mol×K	617.43	Joback Method
cpg	437.76	J/mol×K	650.30	Joback Method
cpg	450.28	J/mol×K	683.18	Joback Method
cpg	462.10	J/mol×K	716.06	Joback Method
cpg	473.22	J/mol×K	748.93	Joback Method
cpg	483.66	J/mol×K	781.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360553&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