2,5-Difluorobenzoic acid, isohexyl ester

Inchi: InChI=1S/C13H16F2O2/c1-9(2)4-3-7-17-13(16)11-8-10(14)5-6-12(11)15/h5-6,8-9H,3-4,7
InchiKey: NRGBAZSTVYYOMM-UHFFFAOYSA-N
Formula: C13H16F2O2
SMILES: CC(C)CCCOC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 242.26

Physical Properties

Property code	Value	Unit	Source
gf	-474.25	kJ/mol	Joback Method
hf	-740.36	kJ/mol	Joback Method
hfus	28.11	kJ/mol	Joback Method
hvap	55.27	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.558		Crippen Method
mcvol	181.250	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1528.00		NIST Webbook
rinpol	1528.00		NIST Webbook
tb	607.87	K	Joback Method
tc	799.01	K	Joback Method
tf	346.07	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.33	J/mol×K	607.87	Joback Method
cpg	473.63	J/mol×K	639.73	Joback Method
cpg	487.21	J/mol×K	671.58	Joback Method
cpg	500.06	J/mol×K	703.44	Joback Method
cpg	512.21	J/mol×K	735.30	Joback Method
cpg	523.67	J/mol×K	767.15	Joback Method
cpg	534.45	J/mol×K	799.01	Joback Method

Sources

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=U338804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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