2,6-Difluorobenzoic acid, hexyl ester

Inchi: InChI=1S/C13H16F2O2/c1-2-3-4-5-9-17-13(16)12-10(14)7-6-8-11(12)15/h6-8H,2-5,9H2,
InchiKey: GPRXOAISRWZXTF-UHFFFAOYSA-N
Formula: C13H16F2O2
SMILES: CCCCCCOC(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 242.26

Physical Properties

Property code	Value	Unit	Source
gf	-471.81	kJ/mol	Joback Method
hf	-735.08	kJ/mol	Joback Method
hfus	31.64	kJ/mol	Joback Method
hvap	55.65	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.702		Crippen Method
mcvol	181.250	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1568.50		NIST Webbook
tb	608.31	K	Joback Method
tc	796.03	K	Joback Method
tf	361.07	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.91	J/mol×K	608.31	Joback Method
cpg	472.91	J/mol×K	639.60	Joback Method
cpg	486.22	J/mol×K	670.88	Joback Method
cpg	498.84	J/mol×K	702.17	Joback Method
cpg	510.79	J/mol×K	733.46	Joback Method
cpg	522.08	J/mol×K	764.74	Joback Method
cpg	532.72	J/mol×K	796.03	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=U292390&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