3,4-Difluorobenzoic acid, undecyl ester

Inchi: InChI=1S/C18H26F2O2/c1-2-3-4-5-6-7-8-9-10-13-22-18(21)15-11-12-16(19)17(20)14-15
InchiKey: SNVHBAADEQJYIC-UHFFFAOYSA-N
Formula: C18H26F2O2
SMILES: CCCCCCCCCCCOC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 312.39

Physical Properties

Property code	Value	Unit	Source
gf	-429.71	kJ/mol	Joback Method
hf	-838.28	kJ/mol	Joback Method
hfus	44.59	kJ/mol	Joback Method
hvap	66.78	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.652		Crippen Method
mcvol	251.700	ml/mol	McGowan Method
pc	1382.99	kPa	Joback Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
tb	722.71	K	Joback Method
tc	904.96	K	Joback Method
tf	417.42	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.89	J/mol×K	722.71	Joback Method
cpg	742.27	J/mol×K	753.09	Joback Method
cpg	757.78	J/mol×K	783.46	Joback Method
cpg	772.44	J/mol×K	813.84	Joback Method
cpg	786.27	J/mol×K	844.21	Joback Method
cpg	799.30	J/mol×K	874.59	Joback Method
cpg	811.54	J/mol×K	904.96	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=U338867&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