Isophthalic acid, 3,5-difluorophenyl pentyl ester

Inchi: InChI=1S/C19H18F2O4/c1-2-3-4-8-24-18(22)13-6-5-7-14(9-13)19(23)25-17-11-15(20)10

InchiKey: AWIVKAIDODABDA-UHFFFAOYSA-N

Formula: C19H18F2O4

SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2cc(F)cc(F)c2)c1

Mol. weight [g/mol]: 348.34

Physical Properties

Property code	Value	Unit	Source
gf	-552.43	kJ/mol	Joback Method
hf	-878.66	kJ/mol	Joback Method
hfus	43.61	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	4.531		Crippen Method
mcvol	249.470	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	2461.00		NIST Webbook
rinpol	2461.00		NIST Webbook
tb	853.54	K	Joback Method
tc	1067.78	K	Joback Method
tf	539.79	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.86	J/mol×K	853.54	Joback Method
cpg	749.74	J/mol×K	889.25	Joback Method
cpg	761.49	J/mol×K	924.95	Joback Method
cpg	772.12	J/mol×K	960.66	Joback Method
cpg	781.65	J/mol×K	996.37	Joback Method
cpg	790.12	J/mol×K	1032.08	Joback Method
cpg	797.53	J/mol×K	1067.78	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=U344371&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