Isophthalic acid, 3,5-difluorophenyl heptyl ester

Inchi: InChI=1S/C21H22F2O4/c1-2-3-4-5-6-10-26-20(24)15-8-7-9-16(11-15)21(25)27-19-13-17

InchiKey: FRNQOQKWWXPWLF-UHFFFAOYSA-N

Formula: C21H22F2O4

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

Mol. weight [g/mol]: 376.39

Physical Properties

Property code	Value	Unit	Source
gf	-535.59	kJ/mol	Joback Method
hf	-919.94	kJ/mol	Joback Method
hfus	48.79	kJ/mol	Joback Method
hvap	85.56	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	5.311		Crippen Method
mcvol	277.650	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook
tb	899.30	K	Joback Method
tc	1113.11	K	Joback Method
tf	562.33	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.53	J/mol×K	899.30	Joback Method
cpg	864.74	J/mol×K	934.94	Joback Method
cpg	876.73	J/mol×K	970.57	Joback Method
cpg	887.55	J/mol×K	1006.21	Joback Method
cpg	897.20	J/mol×K	1041.84	Joback Method
cpg	905.72	J/mol×K	1077.48	Joback Method
cpg	913.14	J/mol×K	1113.11	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=U344374&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