Isophthalic acid, 3,5-difluorophenyl octyl ester

Inchi: InChI=1S/C22H24F2O4/c1-2-3-4-5-6-7-11-27-21(25)16-9-8-10-17(12-16)22(26)28-20-14
InchiKey: DPSWMBLFNHKBSO-UHFFFAOYSA-N
Formula: C22H24F2O4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(F)cc(F)c2)c1
Mol. weight [g/mol]: 390.42

Physical Properties

Property code	Value	Unit	Source
gf	-527.17	kJ/mol	Joback Method
hf	-940.58	kJ/mol	Joback Method
hfus	51.38	kJ/mol	Joback Method
hvap	87.78	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	5.701		Crippen Method
mcvol	291.740	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	2774.00		NIST Webbook
tb	922.18	K	Joback Method
tc	1136.92	K	Joback Method
tf	573.60	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.92	J/mol×K	922.18	Joback Method
cpg	923.26	J/mol×K	957.97	Joback Method
cpg	935.36	J/mol×K	993.76	Joback Method
cpg	946.22	J/mol×K	1029.55	Joback Method
cpg	955.89	J/mol×K	1065.34	Joback Method
cpg	964.40	J/mol×K	1101.13	Joback Method
cpg	971.77	J/mol×K	1136.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344375&Units=SI
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

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