Isophthalic acid, 3,5-difluorophenyl isohexyl ester

Inchi: InChI=1S/C20H20F2O4/c1-13(2)5-4-8-25-19(23)14-6-3-7-15(9-14)20(24)26-18-11-16(21
InchiKey: YAMMGDWPWBWKFV-UHFFFAOYSA-N
Formula: C20H20F2O4
SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)Oc2cc(F)cc(F)c2)c1
Mol. weight [g/mol]: 362.37

Physical Properties

Property code	Value	Unit	Source
gf	-546.45	kJ/mol	Joback Method
hf	-904.58	kJ/mol	Joback Method
hfus	42.68	kJ/mol	Joback Method
hvap	82.94	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	4.777		Crippen Method
mcvol	263.560	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2515.00		NIST Webbook
rinpol	2515.00		NIST Webbook
tb	875.98	K	Joback Method
tc	1091.86	K	Joback Method
tf	536.06	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.36	J/mol×K	875.98	Joback Method
cpg	807.53	J/mol×K	911.96	Joback Method
cpg	819.48	J/mol×K	947.94	Joback Method
cpg	830.25	J/mol×K	983.92	Joback Method
cpg	839.87	J/mol×K	1019.90	Joback Method
cpg	848.34	J/mol×K	1055.88	Joback Method
cpg	855.71	J/mol×K	1091.86	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=U344372&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