Isophthalic acid, di(3,5-difluorophenyl) ester

Inchi: InChI=1S/C20H10F4O4/c21-13-5-14(22)8-17(7-13)27-19(25)11-2-1-3-12(4-11)20(26)28-
InchiKey: MPMAROPAUILXGC-UHFFFAOYSA-N
Formula: C20H10F4O4
SMILES: O=C(Oc1cc(F)cc(F)c1)c1cccc(C(=O)Oc2cc(F)cc(F)c2)c1
Mol. weight [g/mol]: 390.28

Physical Properties

Property code	Value	Unit	Source
gf	-840.48	kJ/mol	Joback Method
hf	-1077.93	kJ/mol	Joback Method
hfus	45.63	kJ/mol	Joback Method
hvap	85.30	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	4.681		Crippen Method
mcvol	243.340	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	2719.00		NIST Webbook
rinpol	2719.00		NIST Webbook
tb	911.60	K	Joback Method
tc	1140.42	K	Joback Method
tf	603.70	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.00	J/mol×K	911.60	Joback Method
cpg	712.73	J/mol×K	949.74	Joback Method
cpg	721.24	J/mol×K	987.87	Joback Method
cpg	728.55	J/mol×K	1026.01	Joback Method
cpg	734.69	J/mol×K	1064.15	Joback Method
cpg	739.68	J/mol×K	1102.28	Joback Method
cpg	743.56	J/mol×K	1140.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344381&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