Isophthalic acid, di(2-bromo-4-fluorophenyl) ester

Inchi: InChI=1S/C20H10Br2F2O4/c21-15-9-13(23)4-6-17(15)27-19(25)11-2-1-3-12(8-11)20(26)
InchiKey: POIQAXWSOPLECQ-UHFFFAOYSA-N
Formula: C20H10Br2F2O4
SMILES: O=C(Oc1ccc(F)cc1Br)c1cccc(C(=O)Oc2ccc(F)cc2Br)c1
Mol. weight [g/mol]: 512.10

Physical Properties

Property code	Value	Unit	Source
gf	-422.22	kJ/mol	Joback Method
hf	-633.05	kJ/mol	Joback Method
hfus	50.04	kJ/mol	Joback Method
hvap	99.80	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	5.928		Crippen Method
mcvol	274.800	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	3296.00		NIST Webbook
rinpol	3296.00		NIST Webbook
tb	1045.38	K	Joback Method
tc	1305.91	K	Joback Method
tf	722.12	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.12	J/mol×K	1045.38	Joback Method
cpg	742.91	J/mol×K	1088.80	Joback Method
cpg	748.52	J/mol×K	1132.22	Joback Method
cpg	753.02	J/mol×K	1175.65	Joback Method
cpg	756.47	J/mol×K	1219.07	Joback Method
cpg	758.93	J/mol×K	1262.49	Joback Method
cpg	760.47	J/mol×K	1305.91	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=U344404&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