Isophthalic acid, di(2-fluorophenyl) ester

Inchi: InChI=1S/C20H12F2O4/c21-15-8-1-3-10-17(15)25-19(23)13-6-5-7-14(12-13)20(24)26-18
InchiKey: NDNOMZDYMUNYFI-UHFFFAOYSA-N
Formula: C20H12F2O4
SMILES: O=C(Oc1ccccc1F)c1cccc(C(=O)Oc2ccccc2F)c1
Mol. weight [g/mol]: 354.30

Physical Properties

Property code	Value	Unit	Source
gf	-431.60	kJ/mol	Joback Method
hf	-662.77	kJ/mol	Joback Method
hfus	40.25	kJ/mol	Joback Method
hvap	85.61	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	4.403		Crippen Method
mcvol	239.800	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	2852.00		NIST Webbook
rinpol	2852.00		NIST Webbook
tb	903.10	K	Joback Method
tc	1144.49	K	Joback Method
tf	577.48	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.87	J/mol×K	903.10	Joback Method
cpg	702.67	J/mol×K	943.33	Joback Method
cpg	712.14	J/mol×K	983.56	Joback Method
cpg	720.31	J/mol×K	1023.80	Joback Method
cpg	727.24	J/mol×K	1064.03	Joback Method
cpg	732.95	J/mol×K	1104.26	Joback Method
cpg	737.51	J/mol×K	1144.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344664&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

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