1,2-Cyclohexanedicarboxylic acid, di(2-fluorophenyl) ester

Inchi: InChI=1S/C20H18F2O4/c21-15-9-3-5-11-17(15)25-19(23)13-7-1-2-8-14(13)20(24)26-18-
InchiKey: QNXVFPFFTYLLTG-UHFFFAOYSA-N
Formula: C20H18F2O4
SMILES: O=C(Oc1ccccc1F)C1CCCCC1C(=O)Oc1ccccc1F
Mol. weight [g/mol]: 360.35

Physical Properties

Property code	Value	Unit	Source
gf	-517.64	kJ/mol	Joback Method
hf	-853.85	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	82.79	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.282		Crippen Method
mcvol	252.700	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	2553.00		NIST Webbook
rinpol	2553.00		NIST Webbook
tb	886.32	K	Joback Method
tc	1121.82	K	Joback Method
tf	541.68	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.66	J/mol×K	886.32	Joback Method
cpg	806.73	J/mol×K	925.57	Joback Method
cpg	819.16	J/mol×K	964.82	Joback Method
cpg	829.98	J/mol×K	1004.07	Joback Method
cpg	839.22	J/mol×K	1043.32	Joback Method
cpg	846.91	J/mol×K	1082.57	Joback Method
cpg	853.10	J/mol×K	1121.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339789&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