1,2-Cyclohexanedicarboxylic acid, 2-fluorophenyl isohexyl ester

Inchi: InChI=1S/C20H27FO4/c1-14(2)8-7-13-24-19(22)15-9-3-4-10-16(15)20(23)25-18-12-6-5-1

InchiKey: DTRNYKHZJCXWGP-UHFFFAOYSA-N

Formula: C20H27FO4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1F

Mol. weight [g/mol]: 350.42

Physical Properties

Property code	Value	Unit	Source
gf	-428.05	kJ/mol	Joback Method
hf	-888.08	kJ/mol	Joback Method
hfus	39.24	kJ/mol	Joback Method
hvap	80.28	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.517		Crippen Method
mcvol	274.690	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	2369.00		NIST Webbook
tb	854.95	K	Joback Method
tc	1070.48	K	Joback Method
tf	487.15	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.63	J/mol×K	854.95	Joback Method
cpg	901.59	J/mol×K	890.87	Joback Method
cpg	917.04	J/mol×K	926.79	Joback Method
cpg	931.01	J/mol×K	962.71	Joback Method
cpg	943.52	J/mol×K	998.64	Joback Method
cpg	954.59	J/mol×K	1034.56	Joback Method
cpg	964.26	J/mol×K	1070.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339783&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

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