1,2-Cyclohexanedicarboxylic acid, 3-fluorophenyl hexyl ester

Inchi: InChI=1S/C20H27FO4/c1-2-3-4-7-13-24-19(22)17-11-5-6-12-18(17)20(23)25-16-10-8-9-1

InchiKey: GKRBQWLFVGXZDI-UHFFFAOYSA-N

Formula: C20H27FO4

SMILES: CCCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 350.42

Physical Properties

Property code	Value	Unit	Source
gf	-425.61	kJ/mol	Joback Method
hf	-882.80	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	80.67	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.661		Crippen Method
mcvol	274.690	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2394.00		NIST Webbook
rinpol	2394.00		NIST Webbook
tb	855.39	K	Joback Method
tc	1068.47	K	Joback Method
tf	502.15	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.12	J/mol×K	855.39	Joback Method
cpg	900.90	J/mol×K	890.90	Joback Method
cpg	916.22	J/mol×K	926.42	Joback Method
cpg	930.11	J/mol×K	961.93	Joback Method
cpg	942.58	J/mol×K	997.44	Joback Method
cpg	953.66	J/mol×K	1032.96	Joback Method
cpg	963.37	J/mol×K	1068.47	Joback Method

Sources

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=U339401&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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