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

Inchi: InChI=1S/C22H31FO4/c1-2-3-4-5-6-9-15-26-21(24)19-13-7-8-14-20(19)22(25)27-18-12-1

InchiKey: RMBWDOAYNPQBQY-UHFFFAOYSA-N

Formula: C22H31FO4

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

Mol. weight [g/mol]: 378.48

Physical Properties

Property code	Value	Unit	Source
gf	-408.77	kJ/mol	Joback Method
hf	-924.08	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	85.12	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.441		Crippen Method
mcvol	302.870	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2602.00		NIST Webbook
rinpol	2602.00		NIST Webbook
tb	901.15	K	Joback Method
tc	1114.21	K	Joback Method
tf	524.69	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.94	J/mol×K	901.15	Joback Method
cpg	1020.63	J/mol×K	936.66	Joback Method
cpg	1035.78	J/mol×K	972.17	Joback Method
cpg	1049.43	J/mol×K	1007.68	Joback Method
cpg	1061.61	J/mol×K	1043.19	Joback Method
cpg	1072.33	J/mol×K	1078.70	Joback Method
cpg	1081.64	J/mol×K	1114.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339402&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