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

Inchi: InChI=1S/C25H37FO4/c1-2-3-4-5-6-7-8-9-14-19-29-24(27)20-15-10-11-16-21(20)25(28)3

InchiKey: ODKBUQDUYAWVPP-UHFFFAOYSA-N

Formula: C25H37FO4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1F

Mol. weight [g/mol]: 420.56

Physical Properties

Property code	Value	Unit	Source
gf	-383.51	kJ/mol	Joback Method
hf	-986.00	kJ/mol	Joback Method
hfus	55.72	kJ/mol	Joback Method
hvap	91.80	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	6.611		Crippen Method
mcvol	345.140	ml/mol	McGowan Method
pc	1052.09	kPa	Joback Method
rinpol	2931.00		NIST Webbook
tb	969.79	K	Joback Method
tc	1188.87	K	Joback Method
tf	558.50	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.55	J/mol×K	969.79	Joback Method
cpg	1204.12	J/mol×K	1006.30	Joback Method
cpg	1218.97	J/mol×K	1042.82	Joback Method
cpg	1232.16	J/mol×K	1079.33	Joback Method
cpg	1243.72	J/mol×K	1115.84	Joback Method
cpg	1253.70	J/mol×K	1152.36	Joback Method
cpg	1262.14	J/mol×K	1188.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339787&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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