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

Inchi: InChI=1S/C19H25FO4/c1-2-3-8-13-23-18(21)14-9-4-5-10-15(14)19(22)24-17-12-7-6-11-1

InchiKey: IVEAVGSPXYRGJS-UHFFFAOYSA-N

Formula: C19H25FO4

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

Mol. weight [g/mol]: 336.40

Physical Properties

Property code	Value	Unit	Source
gf	-434.03	kJ/mol	Joback Method
hf	-862.16	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	78.44	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.271		Crippen Method
mcvol	260.600	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2308.00		NIST Webbook
rinpol	2308.00		NIST Webbook
tb	832.51	K	Joback Method
tc	1046.65	K	Joback Method
tf	490.88	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.18	J/mol×K	832.51	Joback Method
cpg	841.99	J/mol×K	868.20	Joback Method
cpg	857.37	J/mol×K	903.89	Joback Method
cpg	871.34	J/mol×K	939.58	Joback Method
cpg	883.92	J/mol×K	975.27	Joback Method
cpg	895.13	J/mol×K	1010.96	Joback Method
cpg	904.99	J/mol×K	1046.65	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=U339782&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