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

Inchi: InChI=1S/C26H39FO4/c1-2-3-4-5-6-7-8-9-10-15-20-30-25(28)21-16-11-12-17-22(21)26(2

InchiKey: LIPLJZNQHDOEQG-UHFFFAOYSA-N

Formula: C26H39FO4

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

Mol. weight [g/mol]: 434.58

Physical Properties

Property code	Value	Unit	Source
gf	-375.09	kJ/mol	Joback Method
hf	-1006.64	kJ/mol	Joback Method
hfus	58.31	kJ/mol	Joback Method
hvap	94.02	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	7.002		Crippen Method
mcvol	359.230	ml/mol	McGowan Method
pc	989.51	kPa	Joback Method
rinpol	3044.00		NIST Webbook
rinpol	3044.00		NIST Webbook
tb	992.67	K	Joback Method
tc	1215.60	K	Joback Method
tf	569.77	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1249.56	J/mol×K	992.67	Joback Method
cpg	1266.11	J/mol×K	1029.82	Joback Method
cpg	1280.86	J/mol×K	1066.98	Joback Method
cpg	1293.87	J/mol×K	1104.13	Joback Method
cpg	1305.18	J/mol×K	1141.29	Joback Method
cpg	1314.85	J/mol×K	1178.44	Joback Method
cpg	1322.93	J/mol×K	1215.60	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=U339788&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