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

Inchi: InChI=1S/C24H35FO4/c1-2-3-4-5-6-7-8-13-18-28-23(26)19-14-9-10-15-20(19)24(27)29-2

InchiKey: RCVJYHJQQZIGFX-UHFFFAOYSA-N

Formula: C24H35FO4

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

Mol. weight [g/mol]: 406.53

Physical Properties

Property code	Value	Unit	Source
gf	-391.93	kJ/mol	Joback Method
hf	-965.36	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	89.57	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.221		Crippen Method
mcvol	331.050	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2816.00		NIST Webbook
rinpol	2816.00		NIST Webbook
tb	946.91	K	Joback Method
tc	1163.10	K	Joback Method
tf	547.23	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.91	J/mol×K	946.91	Joback Method
cpg	1142.51	J/mol×K	982.94	Joback Method
cpg	1157.46	J/mol×K	1018.97	Joback Method
cpg	1170.82	J/mol×K	1055.01	Joback Method
cpg	1182.60	J/mol×K	1091.04	Joback Method
cpg	1192.86	J/mol×K	1127.07	Joback Method
cpg	1201.62	J/mol×K	1163.10	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=U339786&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