1,2-Cyclohexanedicarboxylic acid, dodecyl pentafluorobenzyl ester

Inchi: InChI=1S/C27H37F5O4/c1-2-3-4-5-6-7-8-9-10-13-16-35-26(33)18-14-11-12-15-19(18)27

InchiKey: HWTHXOGHAHGKBG-UHFFFAOYSA-N

Formula: C27H37F5O4

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 520.57

Physical Properties

Property code	Value	Unit	Source
gf	-1184.43	kJ/mol	Joback Method
hf	-1857.60	kJ/mol	Joback Method
hfus	71.66	kJ/mol	Joback Method
hvap	95.63	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	7.696		Crippen Method
mcvol	380.400	ml/mol	McGowan Method
pc	809.37	kPa	Joback Method
rinpol	2953.00		NIST Webbook
rinpol	2953.00		NIST Webbook
tb	1032.55	K	Joback Method
tc	1272.59	K	Joback Method
tf	633.48	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1335.06	J/mol×K	1032.55	Joback Method
cpg	1350.69	J/mol×K	1072.56	Joback Method
cpg	1364.12	J/mol×K	1112.56	Joback Method
cpg	1375.36	J/mol×K	1152.57	Joback Method
cpg	1384.47	J/mol×K	1192.58	Joback Method
cpg	1391.48	J/mol×K	1232.59	Joback Method
cpg	1396.42	J/mol×K	1272.59	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=U339824&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