1,2-Cyclohexanedicarboxylic acid, nonyl pentafluorobenzyl ester

Inchi: InChI=1S/C24H31F5O4/c1-2-3-4-5-6-7-10-13-32-23(30)15-11-8-9-12-16(15)24(31)33-14

InchiKey: SEMOGNQNAXRGMB-UHFFFAOYSA-N

Formula: C24H31F5O4

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

Mol. weight [g/mol]: 478.49

Physical Properties

Property code	Value	Unit	Source
gf	-1209.69	kJ/mol	Joback Method
hf	-1795.68	kJ/mol	Joback Method
hfus	63.89	kJ/mol	Joback Method
hvap	88.95	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	6.526		Crippen Method
mcvol	338.130	ml/mol	McGowan Method
pc	960.29	kPa	Joback Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
tb	963.91	K	Joback Method
tc	1180.51	K	Joback Method
tf	599.67	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.65	J/mol×K	963.91	Joback Method
cpg	1165.91	J/mol×K	1000.01	Joback Method
cpg	1179.47	J/mol×K	1036.11	Joback Method
cpg	1191.33	J/mol×K	1072.21	Joback Method
cpg	1201.52	J/mol×K	1108.31	Joback Method
cpg	1210.05	J/mol×K	1144.41	Joback Method
cpg	1216.93	J/mol×K	1180.51	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=U339822&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