1,2-Cyclohexanedicarboxylic acid, heptyl pentafluorobenzyl ester

Inchi: InChI=1S/C22H27F5O4/c1-2-3-4-5-8-11-30-21(28)13-9-6-7-10-14(13)22(29)31-12-15-16

InchiKey: RSLWBYYETXSLTC-UHFFFAOYSA-N

Formula: C22H27F5O4

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

Mol. weight [g/mol]: 450.44

Physical Properties

Property code	Value	Unit	Source
gf	-1226.53	kJ/mol	Joback Method
hf	-1754.40	kJ/mol	Joback Method
hfus	58.71	kJ/mol	Joback Method
hvap	84.50	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	5.745		Crippen Method
mcvol	309.950	ml/mol	McGowan Method
pc	1085.63	kPa	Joback Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
tb	918.15	K	Joback Method
tc	1124.67	K	Joback Method
tf	577.13	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.50	J/mol×K	918.15	Joback Method
cpg	1044.49	J/mol×K	952.57	Joback Method
cpg	1058.00	J/mol×K	986.99	Joback Method
cpg	1070.05	J/mol×K	1021.41	Joback Method
cpg	1080.64	J/mol×K	1055.83	Joback Method
cpg	1089.78	J/mol×K	1090.25	Joback Method
cpg	1097.48	J/mol×K	1124.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339820&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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