1,2-Cyclohexanedicarboxylic acid, isobutyl pentafluorobenzyl ester

Inchi: InChI=1S/C19H21F5O4/c1-9(2)7-27-18(25)10-5-3-4-6-11(10)19(26)28-8-12-13(20)15(22
InchiKey: KWPNBZBXANGOOP-UHFFFAOYSA-N
Formula: C19H21F5O4
SMILES: CC(C)COC(=O)C1CCCCC1C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 408.36

Physical Properties

Property code	Value	Unit	Source
gf	-1254.23	kJ/mol	Joback Method
hf	-1697.76	kJ/mol	Joback Method
hfus	47.42	kJ/mol	Joback Method
hvap	77.43	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.431		Crippen Method
mcvol	267.680	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	849.07	K	Joback Method
tc	1048.73	K	Joback Method
tf	528.32	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.22	J/mol×K	849.07	Joback Method
cpg	866.84	J/mol×K	882.35	Joback Method
cpg	880.21	J/mol×K	915.62	Joback Method
cpg	892.32	J/mol×K	948.90	Joback Method
cpg	903.19	J/mol×K	982.18	Joback Method
cpg	912.80	J/mol×K	1015.46	Joback Method
cpg	921.16	J/mol×K	1048.73	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=U339815&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