1,2-Cyclohexanedicarboxylic acid, isohexyl pentafluorobenzyl ester

Inchi: InChI=1S/C21H25F5O4/c1-11(2)6-5-9-29-20(27)12-7-3-4-8-13(12)21(28)30-10-14-15(22
InchiKey: QLGOMQFQIQIHSK-UHFFFAOYSA-N
Formula: C21H25F5O4
SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 436.41

Physical Properties

Property code	Value	Unit	Source
gf	-1237.39	kJ/mol	Joback Method
hf	-1739.04	kJ/mol	Joback Method
hfus	52.60	kJ/mol	Joback Method
hvap	81.89	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.211		Crippen Method
mcvol	295.860	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
tb	894.83	K	Joback Method
tc	1098.49	K	Joback Method
tf	550.86	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.13	J/mol×K	894.83	Joback Method
cpg	985.01	J/mol×K	928.77	Joback Method
cpg	998.48	J/mol×K	962.72	Joback Method
cpg	1010.56	J/mol×K	996.66	Joback Method
cpg	1021.25	J/mol×K	1030.61	Joback Method
cpg	1030.55	J/mol×K	1064.55	Joback Method
cpg	1038.47	J/mol×K	1098.49	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=U339818&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