1,2-Cyclohexanedicarboxylic acid, pentafluorobenzyl pentyl ester

Inchi: InChI=1S/C20H23F5O4/c1-2-3-6-9-28-19(26)11-7-4-5-8-12(11)20(27)29-10-13-14(21)16

InchiKey: SFBSWRBZRZXGIN-UHFFFAOYSA-N

Formula: C20H23F5O4

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

Mol. weight [g/mol]: 422.39

Physical Properties

Property code	Value	Unit	Source
gf	-1243.37	kJ/mol	Joback Method
hf	-1713.12	kJ/mol	Joback Method
hfus	53.53	kJ/mol	Joback Method
hvap	80.05	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	4.965		Crippen Method
mcvol	281.770	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	2241.00		NIST Webbook
rinpol	2241.00		NIST Webbook
tb	872.39	K	Joback Method
tc	1072.56	K	Joback Method
tf	554.59	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.35	J/mol×K	872.39	Joback Method
cpg	925.04	J/mol×K	905.75	Joback Method
cpg	938.43	J/mol×K	939.11	Joback Method
cpg	950.53	J/mol×K	972.47	Joback Method
cpg	961.34	J/mol×K	1005.84	Joback Method
cpg	970.86	J/mol×K	1039.20	Joback Method
cpg	979.09	J/mol×K	1072.56	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339817&Units=SI

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