1,2-Cyclohexanedicarboxylic acid, butyl pentafluorobenzyl ester

Inchi: InChI=1S/C19H21F5O4/c1-2-3-8-27-18(25)10-6-4-5-7-11(10)19(26)28-9-12-13(20)15(22
InchiKey: SAFSWIVVEOKMEF-UHFFFAOYSA-N
Formula: C19H21F5O4
SMILES: CCCCOC(=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	-1251.79	kJ/mol	Joback Method
hf	-1692.48	kJ/mol	Joback Method
hfus	50.94	kJ/mol	Joback Method
hvap	77.82	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.575		Crippen Method
mcvol	267.680	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	2149.00		NIST Webbook
rinpol	2149.00		NIST Webbook
tb	849.51	K	Joback Method
tc	1047.74	K	Joback Method
tf	543.32	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.69	J/mol×K	849.51	Joback Method
cpg	866.22	J/mol×K	882.55	Joback Method
cpg	879.52	J/mol×K	915.59	Joback Method
cpg	891.60	J/mol×K	948.63	Joback Method
cpg	902.46	J/mol×K	981.67	Joback Method
cpg	912.09	J/mol×K	1014.70	Joback Method
cpg	920.50	J/mol×K	1047.74	Joback Method

Sources

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=U339816&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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