1,2-Cyclohexanedicarboxylic acid, ethyl pentafluorobenzyl ester

Inchi: InChI=1S/C17H17F5O4/c1-2-25-16(23)8-5-3-4-6-9(8)17(24)26-7-10-11(18)13(20)15(22)1

InchiKey: OAXRYCICPBPTBP-UHFFFAOYSA-N

Formula: C17H17F5O4

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

Mol. weight [g/mol]: 380.31

Physical Properties

Property code	Value	Unit	Source
gf	-1268.63	kJ/mol	Joback Method
hf	-1651.20	kJ/mol	Joback Method
hfus	45.76	kJ/mol	Joback Method
hvap	73.37	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	3.795		Crippen Method
mcvol	239.500	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook
tb	803.75	K	Joback Method
tc	1000.30	K	Joback Method
tf	520.78	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.58	J/mol×K	803.75	Joback Method
cpg	750.72	J/mol×K	836.51	Joback Method
cpg	763.76	J/mol×K	869.27	Joback Method
cpg	775.70	J/mol×K	902.02	Joback Method
cpg	786.53	J/mol×K	934.78	Joback Method
cpg	796.25	J/mol×K	967.54	Joback Method
cpg	804.84	J/mol×K	1000.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339814&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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