1,2-Cyclohexanedicarboxylic acid, hexyl pentafluorobenzyl ester

Inchi: InChI=1S/C21H25F5O4/c1-2-3-4-7-10-29-20(27)12-8-5-6-9-13(12)21(28)30-11-14-15(22
InchiKey: RIQDDLPINIGHDM-UHFFFAOYSA-N
Formula: C21H25F5O4
SMILES: CCCCCCOC(=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	-1234.95	kJ/mol	Joback Method
hf	-1733.76	kJ/mol	Joback Method
hfus	56.12	kJ/mol	Joback Method
hvap	82.27	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.355		Crippen Method
mcvol	295.860	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	2342.00		NIST Webbook
rinpol	2342.00		NIST Webbook
tb	895.27	K	Joback Method
tc	1098.18	K	Joback Method
tf	565.86	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.64	J/mol×K	895.27	Joback Method
cpg	984.49	J/mol×K	929.09	Joback Method
cpg	997.95	J/mol×K	962.91	Joback Method
cpg	1010.04	J/mol×K	996.73	Joback Method
cpg	1020.76	J/mol×K	1030.54	Joback Method
cpg	1030.11	J/mol×K	1064.36	Joback Method
cpg	1038.11	J/mol×K	1098.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339819&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

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