1,2-Cyclohexanedicarboxylic acid, octyl pentafluorobenzyl ester

Inchi: InChI=1S/C23H29F5O4/c1-2-3-4-5-6-9-12-31-22(29)14-10-7-8-11-15(14)23(30)32-13-16
InchiKey: LTGVCBUZBCGJPT-UHFFFAOYSA-N
Formula: C23H29F5O4
SMILES: CCCCCCCCOC(=O)C1CCCCC1C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 464.47

Physical Properties

Property code	Value	Unit	Source
gf	-1218.11	kJ/mol	Joback Method
hf	-1775.04	kJ/mol	Joback Method
hfus	61.30	kJ/mol	Joback Method
hvap	86.72	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	6.135		Crippen Method
mcvol	324.040	ml/mol	McGowan Method
pc	1020.08	kPa	Joback Method
rinpol	2544.00		NIST Webbook
rinpol	2544.00		NIST Webbook
tb	941.03	K	Joback Method
tc	1152.09	K	Joback Method
tf	588.40	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.86	J/mol×K	941.03	Joback Method
cpg	1104.99	J/mol×K	976.21	Joback Method
cpg	1118.53	J/mol×K	1011.38	Joback Method
cpg	1130.50	J/mol×K	1046.56	Joback Method
cpg	1140.92	J/mol×K	1081.74	Joback Method
cpg	1149.78	J/mol×K	1116.91	Joback Method
cpg	1157.12	J/mol×K	1152.09	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=U339821&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