1,2-Cyclohexanedicarboxylic acid, pentafluorobenzyl undecyl ester

Inchi: InChI=1S/C26H35F5O4/c1-2-3-4-5-6-7-8-9-12-15-34-25(32)17-13-10-11-14-18(17)26(33
InchiKey: HWABLODAZPOMNB-UHFFFAOYSA-N
Formula: C26H35F5O4
SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 506.55

Physical Properties

Property code	Value	Unit	Source
gf	-1192.85	kJ/mol	Joback Method
hf	-1836.96	kJ/mol	Joback Method
hfus	69.07	kJ/mol	Joback Method
hvap	93.40	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	7.306		Crippen Method
mcvol	366.310	ml/mol	McGowan Method
pc	855.46	kPa	Joback Method
tb	1009.67	K	Joback Method
tc	1240.68	K	Joback Method
tf	622.21	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1273.31	J/mol×K	1009.67	Joback Method
cpg	1288.82	J/mol×K	1048.17	Joback Method
cpg	1302.32	J/mol×K	1086.67	Joback Method
cpg	1313.83	J/mol×K	1125.18	Joback Method
cpg	1323.38	J/mol×K	1163.68	Joback Method
cpg	1330.99	J/mol×K	1202.18	Joback Method
cpg	1336.70	J/mol×K	1240.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339823&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume