Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 4-(4-methoxyphenyl)cyclohexyl ester

Inchi: InChI=1S/C22H24F8O5/c1-33-15-6-2-13(3-7-15)14-4-8-16(9-5-14)35-18(32)11-10-17(31
InchiKey: NTXOGCPXERMBCU-UHFFFAOYSA-N
Formula: C22H24F8O5
SMILES: COc1ccc(C2CCC(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)CC2)cc1
Mol. weight [g/mol]: 520.41

Physical Properties

Property code	Value	Unit	Source
gf	-1871.36	kJ/mol	Joback Method
hf	-2460.60	kJ/mol	Joback Method
hfus	44.93	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	5.759		Crippen Method
mcvol	321.130	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	2647.00		NIST Webbook
rinpol	2647.00		NIST Webbook
tb	908.33	K	Joback Method
tc	1113.65	K	Joback Method
tf	543.31	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.83	J/mol×K	908.33	Joback Method
cpg	1098.88	J/mol×K	942.55	Joback Method
cpg	1111.62	J/mol×K	976.77	Joback Method
cpg	1123.10	J/mol×K	1010.99	Joback Method
cpg	1133.41	J/mol×K	1045.21	Joback Method
cpg	1142.61	J/mol×K	1079.43	Joback Method
cpg	1150.80	J/mol×K	1113.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390036&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