Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl diphenylmethyl ester

Inchi: InChI=1S/C22H18F8O4/c23-19(24)21(27,28)22(29,30)20(25,26)13-33-16(31)11-12-17(3

InchiKey: QXFPJLSACSVDDU-UHFFFAOYSA-N

Formula: C22H18F8O4

SMILES: O=C(CCC(=O)OC(c1ccccc1)c1ccccc1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 498.36

Physical Properties

Property code	Value	Unit	Source
gf	-1663.50	kJ/mol	Joback Method
hf	-2119.64	kJ/mol	Joback Method
hfus	41.74	kJ/mol	Joback Method
hvap	76.23	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	5.814		Crippen Method
mcvol	302.360	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2342.00		NIST Webbook
rinpol	2342.00		NIST Webbook
tb	892.29	K	Joback Method
tc	1097.90	K	Joback Method
tf	516.84	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.91	J/mol×K	892.29	Joback Method
cpg	971.89	J/mol×K	926.56	Joback Method
cpg	982.89	J/mol×K	960.83	Joback Method
cpg	992.98	J/mol×K	995.10	Joback Method
cpg	1002.30	J/mol×K	1029.36	Joback Method
cpg	1010.93	J/mol×K	1063.63	Joback Method
cpg	1018.98	J/mol×K	1097.90	Joback Method

Sources

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=U390164&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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