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

Inchi: InChI=1S/C16H14F8O5/c1-27-9-3-2-4-10(7-9)29-12(26)6-5-11(25)28-8-14(19,20)16(23,2

InchiKey: FPKBYIKHDYIJQG-UHFFFAOYSA-N

Formula: C16H14F8O5

SMILES: COc1cccc(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1

Mol. weight [g/mol]: 438.27

Physical Properties

Property code	Value	Unit	Source
gf	-1938.62	kJ/mol	Joback Method
hf	-2370.74	kJ/mol	Joback Method
hfus	36.48	kJ/mol	Joback Method
hvap	64.06	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.095		Crippen Method
mcvol	247.450	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	1986.00		NIST Webbook
rinpol	1986.00		NIST Webbook
tb	756.17	K	Joback Method
tc	936.92	K	Joback Method
tf	472.55	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.62	J/mol×K	756.17	Joback Method
cpg	756.52	J/mol×K	786.29	Joback Method
cpg	767.55	J/mol×K	816.42	Joback Method
cpg	777.74	J/mol×K	846.54	Joback Method
cpg	787.14	J/mol×K	876.67	Joback Method
cpg	795.79	J/mol×K	906.79	Joback Method
cpg	803.74	J/mol×K	936.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390975&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume