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

Inchi: InChI=1S/C16H13F9O5/c1-28-10-6-8(17)2-3-9(10)30-12(27)5-4-11(26)29-7-14(20,21)16

InchiKey: FOAVNLRXVBIBOG-UHFFFAOYSA-N

Formula: C16H13F9O5

SMILES: COc1cc(F)ccc1OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 456.26

Physical Properties

Property code	Value	Unit	Source
gf	-2143.06	kJ/mol	Joback Method
hf	-2578.32	kJ/mol	Joback Method
hfus	39.18	kJ/mol	Joback Method
hvap	63.90	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.234		Crippen Method
mcvol	249.220	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	1916.00		NIST Webbook
rinpol	1916.00		NIST Webbook
tb	760.42	K	Joback Method
tc	938.58	K	Joback Method
tf	485.66	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.26	J/mol×K	760.42	Joback Method
cpg	762.76	J/mol×K	790.11	Joback Method
cpg	773.42	J/mol×K	819.81	Joback Method
cpg	783.28	J/mol×K	849.50	Joback Method
cpg	792.38	J/mol×K	879.19	Joback Method
cpg	800.75	J/mol×K	908.89	Joback Method
cpg	808.43	J/mol×K	938.58	Joback Method

Sources

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=U390896&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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