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

Inchi: InChI=1S/C16H13ClF8O5/c1-28-10-6-8(17)2-3-9(10)30-12(27)5-4-11(26)29-7-14(20,21)1

InchiKey: CBAROLWUPDWNSD-UHFFFAOYSA-N

Formula: C16H13ClF8O5

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

Mol. weight [g/mol]: 472.71

Physical Properties

Property code	Value	Unit	Source
gf	-1960.18	kJ/mol	Joback Method
hf	-2397.95	kJ/mol	Joback Method
hfus	40.29	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.748		Crippen Method
mcvol	259.690	ml/mol	McGowan Method
pc	1361.64	kPa	Joback Method
rinpol	2104.00		NIST Webbook
rinpol	2104.00		NIST Webbook
tb	798.58	K	Joback Method
tc	985.80	K	Joback Method
tf	514.99	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.87	J/mol×K	798.58	Joback Method
cpg	778.66	J/mol×K	829.78	Joback Method
cpg	788.59	J/mol×K	860.99	Joback Method
cpg	797.70	J/mol×K	892.19	Joback Method
cpg	806.03	J/mol×K	923.39	Joback Method
cpg	813.64	J/mol×K	954.60	Joback Method
cpg	820.56	J/mol×K	985.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390930&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