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

Inchi: InChI=1S/C16H13ClF8O4/c1-8-2-3-10(9(17)6-8)29-12(27)5-4-11(26)28-7-14(20,21)16(24

InchiKey: XUICZTJCEUEYJJ-UHFFFAOYSA-N

Formula: C16H13ClF8O4

SMILES: Cc1ccc(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c(Cl)c1

Mol. weight [g/mol]: 456.71

Physical Properties

Property code	Value	Unit	Source
gf	-1855.18	kJ/mol	Joback Method
hf	-2265.73	kJ/mol	Joback Method
hfus	39.10	kJ/mol	Joback Method
hvap	66.69	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.048		Crippen Method
mcvol	253.820	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
tb	776.16	K	Joback Method
tc	961.73	K	Joback Method
tf	492.76	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.87	J/mol×K	776.16	Joback Method
cpg	752.92	J/mol×K	807.09	Joback Method
cpg	763.12	J/mol×K	838.02	Joback Method
cpg	772.55	J/mol×K	868.95	Joback Method
cpg	781.24	J/mol×K	899.87	Joback Method
cpg	789.25	J/mol×K	930.80	Joback Method
cpg	796.64	J/mol×K	961.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390210&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