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

Inchi: InChI=1S/C16H11ClF8O5/c17-9-1-2-10(8(5-9)6-26)30-12(28)4-3-11(27)29-7-14(20,21)16

InchiKey: JIHAZZHZZBBRBH-UHFFFAOYSA-N

Formula: C16H11ClF8O5

SMILES: O=Cc1cc(Cl)ccc1OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 470.70

Physical Properties

Property code	Value	Unit	Source
gf	-1954.70	kJ/mol	Joback Method
hf	-2351.31	kJ/mol	Joback Method
hfus	41.39	kJ/mol	Joback Method
hvap	73.41	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.552		Crippen Method
mcvol	255.390	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	824.82	K	Joback Method
tc	1016.81	K	Joback Method
tf	534.76	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.80	J/mol×K	824.82	Joback Method
cpg	762.30	J/mol×K	856.82	Joback Method
cpg	770.99	J/mol×K	888.82	Joback Method
cpg	778.93	J/mol×K	920.82	Joback Method
cpg	786.20	J/mol×K	952.82	Joback Method
cpg	792.83	J/mol×K	984.81	Joback Method
cpg	798.89	J/mol×K	1016.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389916&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